Propyl sulfide

Other names:	(n-C3H7)2S
	1,1'-Thiobispropane
	4-THIAHEPTANE
	DIPROPYL THIOETHER
	Di-n-propyl thioether
	Dipropyl sulfide
	Dipropyl sulphide
	NSC 78429
	Propane, 1,1'-thiobis-
	Propyl monosulfide
	Sulfide, n-propyl-
	di-n-Propyl sulfide
	di-n-propylsulfide
	n-Propyl sulfide
Inchi:	InChI=1S/C6H14S/c1-3-5-7-6-4-2/h3-6H2,1-2H3
InchiKey:	ZERULLAPCVRMCO-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCCSCCC
Mol. weight [g/mol]:	118.24
CAS:	111-47-7

Physical Properties

Property code	Value	Unit	Source
affp	864.70	kJ/mol	NIST Webbook
basg	834.90	kJ/mol	NIST Webbook
chl	-4794.28 ± 0.75	kJ/mol	NIST Webbook
gf	32.76	kJ/mol	Joback Method
hf	-125.20	kJ/mol	NIST Webbook
hfl	-169.80 ± 0.88	kJ/mol	NIST Webbook
hfus	15.43	kJ/mol	Joback Method
hvap	39.50	kJ/mol	NIST Webbook
hvap	44.20	kJ/mol	NIST Webbook
hvap	44.50	kJ/mol	NIST Webbook
hvap	44.23	kJ/mol	NIST Webbook
hvap	44.70 ± 0.80	kJ/mol	NIST Webbook
hvap	44.60	kJ/mol	NIST Webbook
ie	8.34	eV	NIST Webbook

ie	8.30 ± 0.02	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	8.45 ± 0.05	eV	NIST Webbook
ie	10.90	eV	NIST Webbook
log10ws	-2.58		Aqueous Solubility Prediction Method
log10ws	-2.58		Estimated Solubility Method
logp	2.540		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	878.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	891.20		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	891.20		NIST Webbook
rinpol	896.70		NIST Webbook
rinpol	884.80		NIST Webbook
rinpol	887.40		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	888.00		NIST Webbook

rinpol	888.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1093.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1080.50		NIST Webbook
ripol	1069.00		NIST Webbook
sl	338.28	J/mol×K	NIST Webbook
tb	416.00 ± 0.40	K	NIST Webbook
tb	414.70 ± 0.50	K	NIST Webbook
tb	415.60	K	NIST Webbook
tb	414.65 ± 0.50	K	NIST Webbook
tb	415.60 ± 0.50	K	NIST Webbook
tb	412.00 ± 2.00	K	NIST Webbook
tb	415.85 ± 0.20	K	NIST Webbook
tb	414.00 ± 0.50	K	NIST Webbook
tb	414.00 ± 0.50	K	NIST Webbook
tb	416.00	K	NIST Webbook
tb	415.00 ± 2.00	K	NIST Webbook
tc	594.29	K	Joback Method
tf	170.65	K	Aqueous Solubility Prediction Method
tt	170.44 ± 0.03	K	NIST Webbook
tt	170.43 ± 0.05	K	NIST Webbook
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.89	J/mol×K	594.29	Joback Method
cpg	206.46	J/mol×K	405.46	Joback Method
cpg	259.54	J/mol×K	562.82	Joback Method
cpg	249.77	J/mol×K	531.34	Joback Method
cpg	239.58	J/mol×K	499.87	Joback Method
cpg	228.97	J/mol×K	468.40	Joback Method
cpg	217.94	J/mol×K	436.93	Joback Method
cpl	225.48	J/mol×K	298.15	NIST Webbook
cpl	237.90	J/mol×K	300.00	NIST Webbook
hfust	12.14	kJ/mol	170.40	NIST Webbook
hfust	12.13	kJ/mol	170.40	NIST Webbook
hfust	12.14	kJ/mol	170.44	NIST Webbook

hvapt	36.60	kJ/mol	416.00	NIST Webbook
hvapt	40.60	kJ/mol	390.00	NIST Webbook
hvapt	42.90	kJ/mol	362.00	NIST Webbook
sfust	71.24	J/mol×K	170.44	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48928e+01
Coeff. B	-3.68038e+03
Coeff. C	-5.67920e+01
Temperature range (K), min.	308.78
Temperature range (K), max.	440.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02676e+02
Coeff. B	-8.82408e+03
Coeff. C	-1.29840e+01
Coeff. D	8.43544e-06
Temperature range (K), min.	270.15
Temperature range (K), max.	609.73

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111477&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1836

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB: https://www.cheric.org/files/research/kdb/mol/mol1836.mol

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume