Disulfide, dipropyl

Other names:	(n-C3H7S)2
	1-(Propyldisulfanyl)propane
	4,5-Dithiaoctane
	DI-N-PROPYLDISULFIDE
	Dipropyl disulfide
	Dipropyl disulphide
	NSC 75122
	Propyl disulfide
	di-n-Propyl disulfide
	n-Propyl disulfide
Inchi:	InChI=1S/C6H14S2/c1-3-5-7-8-6-4-2/h3-6H2,1-2H3
InchiKey:	ALVPFGSHPUPROW-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CCCSSCCC
Mol. weight [g/mol]:	150.31
CAS:	629-19-6

Physical Properties

Property code	Value	Unit	Source
chl	-5395.06 ± 0.71	kJ/mol	NIST Webbook
gf	65.88	kJ/mol	Joback Method
hf	-117.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-171.50 ± 1.00	kJ/mol	NIST Webbook
hfus	19.56	kJ/mol	Joback Method
hvap	53.14	kJ/mol	NIST Webbook
hvap	53.80 ± 0.10	kJ/mol	NIST Webbook
hvap	53.80	kJ/mol	NIST Webbook
hvap	54.14 ± 0.42	kJ/mol	NIST Webbook
hvap	54.20	kJ/mol	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	3.188		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1111.00		NIST Webbook

rinpol	1092.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1104.60	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1110.90	NIST Webbook
rinpol	1118.40	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1083.90	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1096.00	NIST Webbook
ripol	1378.00	NIST Webbook
ripol	1375.00	NIST Webbook
ripol	1377.00	NIST Webbook
ripol	1375.00	NIST Webbook
ripol	1418.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1377.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1375.00	NIST Webbook

ripol	1413.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1378.00		NIST Webbook
sl	373.55	J/mol×K	NIST Webbook
tb	468.00 ± 1.70	K	NIST Webbook
tb	468.70	K	NIST Webbook
tc	686.46	K	Joback Method
tf	187.60 ± 0.20	K	NIST Webbook
tt	187.66 ± 0.01	K	NIST Webbook
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.13	J/mol×K	651.09	Joback Method
cpg	254.01	J/mol×K	474.24	Joback Method
cpg	266.31	J/mol×K	509.61	Joback Method
cpg	278.07	J/mol×K	544.98	Joback Method
cpg	289.29	J/mol×K	580.35	Joback Method
cpg	299.98	J/mol×K	615.72	Joback Method
cpg	319.76	J/mol×K	686.46	Joback Method
cpl	262.46	J/mol×K	298.15	NIST Webbook
hfust	13.81	kJ/mol	187.70	NIST Webbook
hfust	13.81	kJ/mol	187.66	NIST Webbook
hfust	13.81	kJ/mol	187.70	NIST Webbook
hvapt	46.60	kJ/mol	425.50	NIST Webbook
hvapt	47.80	kJ/mol	426.50	NIST Webbook
hvapt	47.00	kJ/mol	418.00	NIST Webbook
sfust	73.57	J/mol×K	187.66	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35944e+01
Coeff. B	-3.36629e+03
Coeff. C	-9.36720e+01
Temperature range (K), min.	346.65
Temperature range (K), max.	500.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.10903e+02
Coeff. B	-1.03145e+04
Coeff. C	-1.39703e+01
Coeff. D	7.43052e-06
Temperature range (K), min.	346.15
Temperature range (K), max.	501.15

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1839.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629196&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=1839

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

Legend

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