Butane, 1-(propylthio)-

Other names:	4-Thiaoctane
	Butyl propyl sulfide
	Propyl butyl sulfide
	Sulfide, butyl propyl
Inchi:	InChI=1S/C7H16S/c1-3-5-7-8-6-4-2/h3-7H2,1-2H3
InchiKey:	ZBRWJPVULTZZCE-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCCSCCC
Mol. weight [g/mol]:	132.27
CAS:	1613-46-3

Physical Properties

Property code	Value	Unit	Source
gf	41.18	kJ/mol	Joback Method
hf	-145.94	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	37.99	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.930		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1173.30		NIST Webbook
ripol	1178.20		NIST Webbook
ripol	1178.20		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1196.00		NIST Webbook
tb	431.00 ± 3.00	K	NIST Webbook
tc	615.63	K	Joback Method
tf	203.05	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.59	J/mol×K	428.34	Joback Method
cpg	258.33	J/mol×K	459.56	Joback Method
cpg	270.58	J/mol×K	490.77	Joback Method
cpg	282.33	J/mol×K	521.99	Joback Method
cpg	293.61	J/mol×K	553.20	Joback Method
cpg	304.41	J/mol×K	584.42	Joback Method
cpg	314.75	J/mol×K	615.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48294e+01
Coeff. B	-3.77843e+03
Coeff. C	-6.09680e+01
Temperature range (K), min.	320.80
Temperature range (K), max.	457.95

Sources

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613463&Units=SI

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

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume