Butane, 1-(ethylthio)-

Other names:	1-(Ethylthio)butane
	3-Thiaheptane
	Butyl ethyl sulfide
	Ethyl butyl sulfide
	Ethyl butyl sulphide
	Ethyl n-butyl sulfide
	Sulfide, butyl ethyl
	n-Butylethylsulfide
Inchi:	InChI=1S/C6H14S/c1-3-5-6-7-4-2/h3-6H2,1-2H3
InchiKey:	XJIRSLHMKBUGMR-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCCCSCC
Mol. weight [g/mol]:	118.24
CAS:	638-46-0

Physical Properties

Property code	Value	Unit	Source
chl	-4791.80 ± 1.90	kJ/mol	NIST Webbook
gf	32.76	kJ/mol	Joback Method
hf	-127.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-172.00 ± 2.00	kJ/mol	NIST Webbook
hfus	15.43	kJ/mol	Joback Method
hvap	45.00 ± 1.00	kJ/mol	NIST Webbook
hvap	44.50	kJ/mol	NIST Webbook
hvap	44.90	kJ/mol	NIST Webbook
hvap	45.00	kJ/mol	NIST Webbook
hvap	44.60 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.22		Crippen Method
logp	2.540		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	893.00		NIST Webbook

rinpol	893.00		NIST Webbook
rinpol	892.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1091.10		NIST Webbook
ripol	1096.10		NIST Webbook
ripol	1096.10		NIST Webbook
tb	417.40	K	NIST Webbook
tb	417.00	K	NIST Webbook
tb	417.60 ± 0.40	K	NIST Webbook
tc	594.29	K	Joback Method
tf	178.02 ± 0.10	K	NIST Webbook
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.46	J/mol×K	405.46	Joback Method
cpg	217.94	J/mol×K	436.93	Joback Method
cpg	228.97	J/mol×K	468.40	Joback Method
cpg	239.58	J/mol×K	499.87	Joback Method
cpg	249.77	J/mol×K	531.34	Joback Method
cpg	259.54	J/mol×K	562.82	Joback Method
cpg	268.89	J/mol×K	594.29	Joback Method
hfust	12.39	kJ/mol	178.10	NIST Webbook
hfust	12.39	kJ/mol	178.10	NIST Webbook
hvapt	43.70	kJ/mol	379.50	NIST Webbook
hvapt	40.70	kJ/mol	389.00	NIST Webbook
hvapt	43.50	kJ/mol	332.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48028e+01
Coeff. B	-3.66853e+03

Coeff. C	-5.71900e+01
Temperature range (K), min.	309.93
Temperature range (K), max.	443.71

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638460&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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