Butane, 2-(ethylthio)-

Other names:	(1-Methylpropyl) ethyl sulfide
	2-(Ethylthio)butane
	4-Methyl-3-thiahexane
	Ethyl (1-methylpropyl) sulfide
	Ethyl 2-butyl sulfide
	Sulfide, sec-butyl ethyl
	sec-Butyl ethyl sulfide
Inchi:	InChI=1S/C6H14S/c1-4-6(3)7-5-2/h6H,4-5H2,1-3H3
InchiKey:	JFNGZXUPUVUYST-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCSC(C)CC
Mol. weight [g/mol]:	118.24
CAS:	5008-72-0

Physical Properties

Property code	Value	Unit	Source
gf	30.32	kJ/mol	Joback Method
hf	-130.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.538		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	406.80 ± 0.40	K	NIST Webbook
tc	598.38	K	Joback Method
tf	176.78	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.46	J/mol×K	405.02	Joback Method
cpg	218.30	J/mol×K	437.25	Joback Method
cpg	229.68	J/mol×K	469.47	Joback Method
cpg	240.61	J/mol×K	501.70	Joback Method
cpg	251.08	J/mol×K	533.93	Joback Method
cpg	261.10	J/mol×K	566.16	Joback Method
cpg	270.69	J/mol×K	598.38	Joback Method
hvapt	41.20	kJ/mol	369.00	NIST Webbook
hvapt	39.00	kJ/mol	377.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47793e+01
Coeff. B	-3.58233e+03
Coeff. C	-5.42400e+01
Temperature range (K), min.	301.44
Temperature range (K), max.	432.61

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5008720&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume