Methyl n-butyl disulfide

Other names:	1-(Methyldisulfanyl)butane
	2,3-Diathiaheptane
	2,3-Dithiaheptane
	Butyl methyl disulfide
	Disulfide, butyl methyl
	Methyl butyl disulfide
	Methyl n-butyl disulphide
Inchi:	InChI=1S/C5H12S2/c1-3-4-5-7-6-2/h3-5H2,1-2H3
InchiKey:	ABUPWXCYFWRZKL-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CCCCSSC
Mol. weight [g/mol]:	136.28
CAS:	60779-24-0

Physical Properties

Property code	Value	Unit	Source
gf	57.46	kJ/mol	Joback Method
hf	-62.79	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.36	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.798		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	451.36	K	Joback Method
tc	666.63	K	Joback Method
tf	214.91	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/mol×K	451.36	Joback Method
cpg	224.75	J/mol×K	487.24	Joback Method
cpg	235.26	J/mol×K	523.12	Joback Method
cpg	245.30	J/mol×K	558.99	Joback Method
cpg	254.88	J/mol×K	594.87	Joback Method
cpg	264.00	J/mol×K	630.75	Joback Method
cpg	272.66	J/mol×K	666.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52527e+01
Coeff. B	-4.01255e+03
Coeff. C	-6.64510e+01
Temperature range (K), min.	334.58
Temperature range (K), max.	470.08

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=C60779240&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
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