4-methoxy-2-methyl-2-butanethiol

Other names:	2-Butanethiol, 4-methoxy-2-methyl-
	4-Methoxy-2-methyl-2-mercaptobutane
	4-methoxy-2-methylbutanethiol-2
	4-methoxy-2-methylbutane-2-thiol
Inchi:	InChI=1S/C6H14OS/c1-6(2,8)4-5-7-3/h8H,4-5H2,1-3H3
InchiKey:	XVHGKKGBUDMTIQ-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	COCCC(C)(C)S
Mol. weight [g/mol]:	134.24
CAS:	94087-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-73.13	kJ/mol	Joback Method
hf	-269.66	kJ/mol	Joback Method
hfus	9.11	kJ/mol	Joback Method
hvap	36.80	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.731		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	910.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1216.00		NIST Webbook
tb	418.73	K	Joback Method
tc	619.81	K	Joback Method
tf	218.49	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.73	J/mol×K	418.73	Joback Method
cpg	242.30	J/mol×K	452.24	Joback Method
cpg	254.25	J/mol×K	485.76	Joback Method
cpg	265.60	J/mol×K	519.27	Joback Method
cpg	276.38	J/mol×K	552.78	Joback Method
cpg	286.60	J/mol×K	586.29	Joback Method
cpg	296.29	J/mol×K	619.81	Joback Method

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=C94087839&Units=SI
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
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