2-methyl-3-sulfanyl-butan-1-ol

Other names: 3-mercapto-2-methylbutanol
3-mercapto-2-methyl-1-butanol
Inchi: InChI=1S/C5H12OS/c1-4(3-6)5(2)7/h4-7H,3H2,1-2H3
InchiKey: RFMHFOPFUZZBAD-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CC(S)C(C)CO
Mol. weight [g/mol]: 120.21

Physical Properties

Property code	Value	Unit	Source
gf	-121.09	kJ/mol	Joback Method
hf	-270.84	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.933		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1060.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	467.96	K	Joback Method
tc	658.24	K	Joback Method
tf	213.39	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.56	J/mol×K	467.96	Joback Method
cpg	222.02	J/mol×K	499.67	Joback Method
cpg	231.06	J/mol×K	531.39	Joback Method
cpg	239.68	J/mol×K	563.10	Joback Method
cpg	247.90	J/mol×K	594.82	Joback Method
cpg	255.72	J/mol×K	626.53	Joback Method
cpg	263.16	J/mol×K	658.24	Joback Method

Sources

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=R291995&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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