3-Sulfanyl-2-methylbutan-1-thiol

Inchi: InChI=1S/C5H10OS/c1-4(3-6)5(2)7/h3-5,7H,1-2H3
InchiKey: GLNQOYSTMOFRHJ-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CC(S)C(C)C=O
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-83.79	kJ/mol	Joback Method
hf	-204.19	kJ/mol	Joback Method
hfus	7.99	kJ/mol	Joback Method
hvap	39.41	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.140		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1051.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1780.00		NIST Webbook
tb	424.44	K	Joback Method
tc	631.58	K	Joback Method
tf	194.57	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.53	J/mol×K	424.44	Joback Method
cpg	195.32	J/mol×K	458.96	Joback Method
cpg	204.64	J/mol×K	493.49	Joback Method
cpg	213.49	J/mol×K	528.01	Joback Method
cpg	221.89	J/mol×K	562.54	Joback Method
cpg	229.85	J/mol×K	597.06	Joback Method
cpg	237.38	J/mol×K	631.58	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=R621277&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