1-Mercaptobutan-3-ol

Inchi: InChI=1S/C4H10OS/c1-4(5)2-3-6/h4-6H,2-3H2,1H3
InchiKey: WHGYPRRJIBXGKB-UHFFFAOYSA-N
Formula: C4H10OS
SMILES: CC(O)CCS
Mol. weight [g/mol]: 106.19

Physical Properties

Property code	Value	Unit	Source
gf	-127.07	kJ/mol	Joback Method
hf	-244.92	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.687		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	881.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	881.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1622.00		NIST Webbook
tb	445.52	K	Joback Method
tc	633.53	K	Joback Method
tf	217.12	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.64	J/mol×K	445.52	Joback Method
cpg	181.58	J/mol×K	476.85	Joback Method
cpg	189.18	J/mol×K	508.19	Joback Method
cpg	196.43	J/mol×K	539.52	Joback Method

cpg	203.36	J/mol×K	570.86	Joback Method
cpg	209.97	J/mol×K	602.19	Joback Method
cpg	216.27	J/mol×K	633.53	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=R291935&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