

3-Mercapto-2-ethyl-1-propanol

Inchi:	InChI=1S/C5H12OS/c1-2-5(3-6)4-7/h5-7H,2-4H2,1H3
InchiKey:	WPGXWRDNSGSYBE-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CCC(CO)CS
Mol. weight [g/mol]:	120.21

Physical Properties

Property code	Value	Unit	Source
gf	-118.65	kJ/mol	Joback Method
hf	-265.56	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.935		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1020.00		NIST Webbook
tb	468.40	K	Joback Method
tc	654.54	K	Joback Method
tf	228.39	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.35	J/mol×K	468.40	Joback Method
cpg	221.54	J/mol×K	499.42	Joback Method
cpg	230.32	J/mol×K	530.45	Joback Method
cpg	238.70	J/mol×K	561.47	Joback Method
cpg	246.71	J/mol×K	592.49	Joback Method
cpg	254.35	J/mol×K	623.52	Joback Method
cpg	261.63	J/mol×K	654.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602909&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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