1-Propanol, 3-[(2-hydroxyethyl)thio]-

Other names: 2-Ethanol 3-propanol sulfide
3-[(2-Hydroxyethyl)sulfanyl]-1-propanol
2-Hydroxyethyl 3-hydroxypropyl sulfide
Inchi: InChI=1S/C5H12O2S/c6-2-1-4-8-5-3-7/h6-7H,1-5H2
InchiKey: YJGRQEWXDDCCCV-UHFFFAOYSA-N
Formula: C5H12O2S
SMILES: OCCCSCCO
Mol. weight [g/mol]: 136.21
CAS: 5323-60-4

Physical Properties

Property code	Value	Unit	Source
gf	-249.30	kJ/mol	Joback Method
hf	-409.12	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.094		Crippen Method
mcvol	109.400	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
tb	566.94	K	Joback Method
tc	741.23	K	Joback Method
tf	302.15	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.29	J/mol×K	566.94	Joback Method
cpg	264.12	J/mol×K	595.99	Joback Method
cpg	271.62	J/mol×K	625.04	Joback Method
cpg	278.79	J/mol×K	654.08	Joback Method

cpg	285.64	J/mol×K	683.13	Joback Method
cpg	292.17	J/mol×K	712.18	Joback Method
cpg	298.40	J/mol×K	741.23	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=C5323604&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume