1-Propanol, 3-(ethylthio)-

Other names: 3-Ethylthio-1-propanol
3-(ethylthio)propanol
Inchi: InChI=1S/C5H12OS/c1-2-7-5-3-4-6/h6H,2-5H2,1H3
InchiKey: KRUJXSIEMOWXOF-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CCSCCCO
Mol. weight [g/mol]: 120.21
CAS: 18721-61-4

Physical Properties

Property code	Value	Unit	Source
gf	-112.48	kJ/mol	Joback Method
hf	-256.89	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.122		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
ripol	1802.00		NIST Webbook
ripol	1802.00		NIST Webbook
tb	474.76	K	Joback Method
tc	656.94	K	Joback Method
tf	241.33	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.57	J/mol×K	474.76	Joback Method
cpg	222.54	J/mol×K	505.12	Joback Method
cpg	231.16	J/mol×K	535.49	Joback Method
cpg	239.43	J/mol×K	565.85	Joback Method
cpg	247.36	J/mol×K	596.22	Joback Method

cpg	254.95	J/mol×K	626.58	Joback Method
cpg	262.20	J/mol×K	656.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18721614&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume