3-(allylthio)propanol

Inchi: InChI=1S/C6H12OS/c1-2-5-8-6-3-4-7/h2,7H,1,3-6H2
InchiKey: HTKIDHNLOHZPEP-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: C=CCSCCCO
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-16.22	kJ/mol	Joback Method
hf	-152.10	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.288		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
rinpol	1052.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1052.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	494.32	K	Joback Method
tc	678.29	K	Joback Method
tf	250.84	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.20	J/mol×K	494.32	Joback Method
cpg	246.62	J/mol×K	524.98	Joback Method
cpg	255.61	J/mol×K	555.64	Joback Method
cpg	264.20	J/mol×K	586.30	Joback Method
cpg	272.40	J/mol×K	616.97	Joback Method

cpg	280.21	J/mol×K	647.63	Joback Method
cpg	287.64	J/mol×K	678.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222390&Units=SI

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