1-Propanol, 3-mercapto-

Other names:	1-mercapto-3-propanol
	3-mercaptopropanol
	3-Mercapto-1-propanol
Inchi:	InChI=1S/C3H8OS/c4-2-1-3-5/h4-5H,1-3H2
InchiKey:	SHLSSLVZXJBVHE-UHFFFAOYSA-N
Formula:	C3H8OS
SMILES:	OCCCS
Mol. weight [g/mol]:	92.16
CAS:	19721-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-133.05	kJ/mol	Joback Method
hf	-219.00	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	45.69	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.299		Crippen Method
mcvol	75.350	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	840.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1620.00		NIST Webbook
tb	423.08	K	Joback Method
tc	608.50	K	Joback Method
tf	220.85	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.08	J/mol×K	423.08	Joback Method
cpg	143.40	J/mol×K	453.98	Joback Method
cpg	149.46	J/mol×K	484.89	Joback Method
cpg	155.26	J/mol×K	515.79	Joback Method
cpg	160.82	J/mol×K	546.69	Joback Method
cpg	166.13	J/mol×K	577.60	Joback Method
cpg	171.20	J/mol×K	608.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19721223&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
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