

1-mercapto-3-pentanol

Other names:	1-mercaptopentan-3-ol
Inchi:	InChI=1S/C5H12OS/c1-2-5(6)3-4-7/h5-7H,2-4H2,1H3
InchiKey:	JCNWZSMCAXWBGZ-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CCC(O)CCS
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	-1.36		Crippen Method
logp	1.077		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	981.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	981.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	468.40	K	Joback Method
tc	654.54	K	Joback Method
tf	228.39	K	Joback Method
vc	0.383	m ³ /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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R291955&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

Latest version available from:

<https://www.chemeo.com/cid/80-855-4/1-mercapto-3-pentanol.pdf>

Generated by Cheméo on 2024-04-28 07:00:17.952966638 +0000 UTC m=+16576866.873543953.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.