

3-(methylthio) hexanol

Other names:	3-Methylthio-1-hexanol 3-(Methylthio)-hexan-1-ol
Inchi:	InChI=1S/C7H16OS/c1-3-4-7(9-2)5-6-8/h7-8H,3-6H2,1-2H3
InchiKey:	JSASXSHMJYRPCM-UHFFFAOYSA-N
Formula:	C7H16OS
SMILES:	CCCC(CCO)SC
Mol. weight [g/mol]:	148.27
CAS:	51755-66-9

Physical Properties

Property code	Value	Unit	Source
gf	-98.08	kJ/mol	Joback Method
hf	-303.45	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.901		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1203.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1843.00		NIST Webbook
tb	520.08	K	Joback Method
tc	702.37	K	Joback Method
tf	248.87	K	Joback Method
vc	0.494	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.21	J/mol×K	520.08	Joback Method
cpg	309.58	J/mol×K	550.46	Joback Method

cpg	320.47	J/mol×K	580.84	Joback Method
cpg	330.88	J/mol×K	611.22	Joback Method
cpg	340.83	J/mol×K	641.61	Joback Method
cpg	350.33	J/mol×K	671.99	Joback Method
cpg	359.37	J/mol×K	702.37	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=C51755669&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
r ipol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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