3-(Methylthio)-hexan-1-ol

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

Physical Properties

Property code	Value	Unit	Source
hfus	18.58	kJ/mol	Joback Method
logp	1.901		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
rinpol	1203.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1843.00		NIST Webbook
tb	498.41	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51755669&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature