3-Mercaptohexyl acetate

Other names:	3-sulfanylhexyl acetate
	1-Hexanol, 3-mercapto-, 1-acetate
Inchi:	InChI=1S/C8H16O2S/c1-3-4-8(11)5-6-10-7(2)9/h8,11H,3-6H2,1-2H3
InchiKey:	JUCARGIKESIVLB-UHFFFAOYSA-N
Formula:	C8H16O2S
SMILES:	CCCC(S)CCOC(C)=O
Mol. weight [g/mol]:	176.28
CAS:	136954-20-6

Physical Properties

Property code	Value	Unit	Source
gf	-190.49	kJ/mol	Joback Method
hf	-420.05	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.038		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1252.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1740.00		NIST Webbook
tb	521.15	K	Joback Method

tc	719.67	K	Joback Method
tf	273.54	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.65	J/mol×K	521.15	Joback Method
cpg	342.79	J/mol×K	554.24	Joback Method
cpg	355.36	J/mol×K	587.32	Joback Method
cpg	367.34	J/mol×K	620.41	Joback Method
cpg	378.76	J/mol×K	653.50	Joback Method
cpg	389.62	J/mol×K	686.59	Joback Method
cpg	399.91	J/mol×K	719.67	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=C136954206&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

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