2-Mercaptohexyl-4-acetate

Inchi: InChI=1S/C8H16O2S/c1-4-8(5-6(2)11)10-7(3)9/h6,8,11H,4-5H2,1-3H3
InchiKey: JVSSZFATQMMTDW-UHFFFAOYSA-N
Formula: C8H16O2S
SMILES: CCC(CC(C)S)OC(C)=O
Mol. weight [g/mol]: 176.28

Physical Properties

Property code	Value	Unit	Source
gf	-192.93	kJ/mol	Joback Method
hf	-425.33	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.036		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1578.00		NIST Webbook
tb	520.71	K	Joback Method
tc	723.56	K	Joback Method
tf	258.54	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.93	J/mol×K	520.71	Joback Method
cpg	343.43	J/mol×K	554.52	Joback Method

cpg	356.32	J/mol×K	588.33	Joback Method
cpg	368.60	J/mol×K	622.14	Joback Method
cpg	380.27	J/mol×K	655.94	Joback Method
cpg	391.34	J/mol×K	689.75	Joback Method
cpg	401.82	J/mol×K	723.56	Joback Method

Sources

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=R291742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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