3-mercapto-2-methylpentyl-acetate

Inchi: InChI=1S/C8H16O2S/c1-4-8(11)6(2)5-10-7(3)9/h6,8,11H,4-5H2,1-3H3
InchiKey: RVVSZQSNXSLHMC-UHFFFAOYSA-N
Formula: C8H16O2S
SMILES: CCC(S)C(C)COC(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	-1.98		Crippen Method
logp	1.894		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1207.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1687.00		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

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=R291782&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
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