4-Mercapto-3-methylpentyl-2-acetate

Inchi: InChI=1S/C8H16O2S/c1-5(7(3)11)6(2)10-8(4)9/h5-7,11H,1-4H3
InchiKey: HQPZOLJRLYJHKW-UHFFFAOYSA-N
Formula: C8H16O2S
SMILES: CC(=O)OC(C)C(C)C(C)S
Mol. weight [g/mol]: 176.28

Physical Properties

Property code	Value	Unit	Source
gf	-195.37	kJ/mol	Joback Method
hf	-430.61	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	48.13	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.892		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1613.00		NIST Webbook
tb	520.27	K	Joback Method
tc	727.60	K	Joback Method
tf	243.54	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.21	J/mol×K	520.27	Joback Method
cpg	344.08	J/mol×K	554.83	Joback Method
cpg	357.30	J/mol×K	589.38	Joback Method
cpg	369.88	J/mol×K	623.94	Joback Method
cpg	381.81	J/mol×K	658.49	Joback Method

cpg	393.11	J/mol×K	693.05	Joback Method
cpg	403.78	J/mol×K	727.60	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=R291851&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