4-Mercapto-4-methylpentyl-2-acetate

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

Physical Properties

Property code	Value	Unit	Source
gf	-187.65	kJ/mol	Joback Method
hf	-428.80	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	47.61	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.036		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1518.00		NIST Webbook
tb	517.92	K	Joback Method
tc	729.05	K	Joback Method
tf	275.96	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.94	J/mol×K	517.92	Joback Method
cpg	347.09	J/mol×K	553.11	Joback Method
cpg	360.46	J/mol×K	588.30	Joback Method
cpg	373.06	J/mol×K	623.49	Joback Method

cpg	384.92	J/mol×K	658.68	Joback Method
cpg	396.08	J/mol×K	693.87	Joback Method
cpg	406.55	J/mol×K	729.05	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=R291866&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