4-mercaptopentyl-2-acetate

Inchi: InChI=1S/C7H14O2S/c1-5(4-6(2)10)9-7(3)8/h5-6,10H,4H2,1-3H3
InchiKey: VJRLTXOZBKLRSU-UHFFFAOYSA-N
Formula: C7H14O2S
SMILES: CC(=O)OC(C)CC(C)S
Mol. weight [g/mol]: 162.25

Physical Properties

Property code	Value	Unit	Source
gf	-201.35	kJ/mol	Joback Method
hf	-404.69	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.646		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1053.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1531.00		NIST Webbook
tb	497.83	K	Joback Method
tc	703.64	K	Joback Method
tf	247.27	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.07	J/mol×K	497.83	Joback Method
cpg	298.53	J/mol×K	532.13	Joback Method
cpg	310.43	J/mol×K	566.43	Joback Method
cpg	321.79	J/mol×K	600.73	Joback Method
cpg	332.59	J/mol×K	635.03	Joback Method
cpg	342.85	J/mol×K	669.34	Joback Method

cpg	352.57	J/mol×K	703.64	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=R291886&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