1-Mercaptopentyl-3-acetate

Inchi: InChI=1S/C7H14O2S/c1-3-7(4-5-10)9-6(2)8/h7,10H,3-5H2,1-2H3
InchiKey: XYCZHHLYBJAWHY-UHFFFAOYSA-N
Formula: C7H14O2S
SMILES: CCC(CCS)OC(C)=O
Mol. weight [g/mol]: 162.25

Physical Properties

Property code	Value	Unit	Source
gf	-198.91	kJ/mol	Joback Method
hf	-399.41	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.648		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
ripol	1611.00		NIST Webbook
tb	498.27	K	Joback Method
tc	699.54	K	Joback Method
tf	262.27	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.82	J/mol×K	498.27	Joback Method
cpg	297.93	J/mol×K	531.81	Joback Method
cpg	309.52	J/mol×K	565.36	Joback Method
cpg	320.59	J/mol×K	598.90	Joback Method
cpg	331.14	J/mol×K	632.45	Joback Method
cpg	341.18	J/mol×K	665.99	Joback Method

cpg	350.72	J/mol×K	699.54	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=R291737&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