4-Mercaptononyl-2-acetate

Inchi: InChI=1S/C11H22O2S/c1-4-5-6-7-11(14)8-9(2)13-10(3)12/h9,11,14H,4-8H2,1-3H3
InchiKey: ATUWCVJQUQRXHL-UHFFFAOYSA-N
Formula: C11H22O2S
SMILES: CCCCCC(S)CC(C)OC(C)=O
Mol. weight [g/mol]: 218.36

Physical Properties

Property code	Value	Unit	Source
gf	-167.67	kJ/mol	Joback Method
hf	-487.25	kJ/mol	Joback Method
hfus	24.03	kJ/mol	Joback Method
hvap	55.20	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.207		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	589.35	K	Joback Method
tc	783.94	K	Joback Method
tf	292.35	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.56	J/mol×K	589.35	Joback Method
cpg	488.44	J/mol×K	621.78	Joback Method
cpg	503.56	J/mol×K	654.21	Joback Method
cpg	517.93	J/mol×K	686.64	Joback Method
cpg	531.56	J/mol×K	719.08	Joback Method

cpg	544.48	J/mol×K	751.51	Joback Method
cpg	556.68	J/mol×K	783.94	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=R291871&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