3-mercaptoheptyl-acetate

Inchi: InChI=1S/C9H18O2S/c1-3-4-5-9(12)6-7-11-8(2)10/h9,12H,3-7H2,1-2H3
InchiKey: JWESHEXXXWDVAQ-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CCCCC(S)CCOC(C)=O
Mol. weight [g/mol]: 190.30

Physical Properties

Property code	Value	Unit	Source
gf	-182.07	kJ/mol	Joback Method
hf	-440.69	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.428		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
ripol	1823.00		NIST Webbook
tb	544.03	K	Joback Method
tc	739.88	K	Joback Method
tf	284.81	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.39	J/mol×K	544.03	Joback Method
cpg	389.44	J/mol×K	576.67	Joback Method
cpg	402.86	J/mol×K	609.31	Joback Method
cpg	415.65	J/mol×K	641.95	Joback Method
cpg	427.82	J/mol×K	674.60	Joback Method
cpg	439.39	J/mol×K	707.24	Joback Method
cpg	450.35	J/mol×K	739.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R291826&Units=SI
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

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