Pentanoic acid, 3-mercaptohexyl ester

Other names: 3-mercaptohexyl pentanoate
Inchi: InChI=1S/C11H22O2S/c1-3-5-7-11(12)13-9-8-10(14)6-4-2/h10,14H,3-9H2,1-2H3
InchiKey: VMHWVDZUYLYJAJ-UHFFFAOYSA-N
Formula: C11H22O2S
SMILES: CCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 218.36

Physical Properties

Property code	Value	Unit	Source
gf	-165.23	kJ/mol	Joback Method
hf	-481.97	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.208		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
tb	589.79	K	Joback Method
tc	780.71	K	Joback Method
tf	307.35	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.19	J/mol×K	589.79	Joback Method
cpg	487.71	J/mol×K	621.61	Joback Method
cpg	502.52	J/mol×K	653.43	Joback Method
cpg	516.61	J/mol×K	685.25	Joback Method
cpg	530.01	J/mol×K	717.07	Joback Method
cpg	542.72	J/mol×K	748.89	Joback Method
cpg	554.75	J/mol×K	780.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U281469&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume