3-Mercaptohexyl hexanoate

Other names: Hexanoic acid, 3-mercaptohexyl ester
3-sulfanylhexyl hexanoate
Inchi: InChI=1S/C12H24O2S/c1-3-5-6-8-12(13)14-10-9-11(15)7-4-2/h11,15H,3-10H2,1-2H3
InchiKey: KVXKOWZLYWBURN-UHFFFAOYSA-N
Formula: C12H24O2S
SMILES: CCCCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]: 232.38
CAS: 136954-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-156.81	kJ/mol	Joback Method
hf	-502.61	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	57.81	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.599		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
ripol	2046.00		NIST Webbook
ripol	2025.00		NIST Webbook
ripol	2046.00		NIST Webbook
tb	612.67	K	Joback Method
tc	801.44	K	Joback Method
tf	318.62	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.04	J/mol×K	612.67	Joback Method
cpg	539.16	J/mol×K	644.13	Joback Method
cpg	554.52	J/mol×K	675.59	Joback Method
cpg	569.14	J/mol×K	707.06	Joback Method

cpg	583.02	J/mol×K	738.52	Joback Method
cpg	596.19	J/mol×K	769.98	Joback Method
cpg	608.65	J/mol×K	801.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136954228&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