Propanoic acid, 3-mercapto-, dodecyl ester

Other names:	Dodecyl 3-mercaptopropionate
	Lauryl «beta»-mercaptopropionate
	Lauryl 3-mercaptopropionate
	Propionic acid, 3-mercapto-, dodecyl ester
Inchi:	InChI=1S/C15H30O2S/c1-2-3-4-5-6-7-8-9-10-11-13-17-15(16)12-14-18/h18H,2-14H2,1H
InchiKey:	ARNIBHATWCFIIK-UHFFFAOYSA-N
Formula:	C15H30O2S
SMILES:	CCCCCCCCCCCCOC(=O)CCS
Mol. weight [g/mol]:	274.46
CAS:	6380-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-129.11	kJ/mol	Joback Method
hf	-559.25	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.770		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
tb	681.75	K	Joback Method
tc	863.36	K	Joback Method
tf	367.43	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.76	J/mol×K	681.75	Joback Method
cpg	700.99	J/mol×K	712.02	Joback Method
cpg	717.40	J/mol×K	742.29	Joback Method
cpg	732.99	J/mol×K	772.56	Joback Method
cpg	747.79	J/mol×K	802.82	Joback Method

cpg	761.82	J/mol×K	833.09	Joback Method
cpg	775.09	J/mol×K	863.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6380718&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume