Octanethioic acid, S-hexyl ester

Other names: Octanethioic acid, hexyl ester
Inchi: InChI=1S/C14H28OS/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h3-13H2,1-2H3
InchiKey: ARKGQSZBBOGCSX-UHFFFAOYSA-N
Formula: C14H28OS
SMILES: CCCCCCCC(=O)SCCCCCC
Mol. weight [g/mol]: 244.44
CAS: 55590-85-7

Physical Properties

Property code	Value	Unit	Source
gf	-28.80	kJ/mol	Joback Method
hf	-403.00	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.187		Crippen Method
mcvol	226.040	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
tb	642.37	K	Joback Method
tc	825.46	K	Joback Method
tf	331.87	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.69	J/mol×K	642.37	Joback Method
cpg	620.82	J/mol×K	672.89	Joback Method
cpg	637.13	J/mol×K	703.40	Joback Method
cpg	652.65	J/mol×K	733.92	Joback Method
cpg	667.39	J/mol×K	764.43	Joback Method
cpg	681.37	J/mol×K	794.95	Joback Method
cpg	694.62	J/mol×K	825.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590857&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