

Hexanoic acid, 3 3,5,5-trimethyl-, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C14H20F8O2/c1-8(6-11(2,3)4)5-9(23)24-7-12(17,18)14(21,22)13(19,20)10(15)
InchiKey: QCHHKNOVZLICRC-UHFFFAOYSA-N
Formula: C14H20F8O2
SMILES: CC(CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC(C)(C)C
Mol. weight [g/mol]: 372.29

Physical Properties

Property code	Value	Unit	Source
gf	-1718.92	kJ/mol	Joback Method
hf	-2191.53	kJ/mol	Joback Method
hfus	22.74	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.163		Crippen Method
mcvol	229.720	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
tb	576.37	K	Joback Method
tc	730.34	K	Joback Method
tf	304.10	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.95	J/molxK	576.37	Joback Method
cpg	658.45	J/molxK	602.03	Joback Method
cpg	673.07	J/molxK	627.69	Joback Method
cpg	686.86	J/molxK	653.35	Joback Method
cpg	699.84	J/molxK	679.01	Joback Method
cpg	712.08	J/molxK	704.68	Joback Method
cpg	723.60	J/molxK	730.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406818&Units=SI

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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