Nonanoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C14H20F8O2/c1-2-3-4-5-6-7-8-10(23)24-9-12(17,18)14(21,22)13(19,20)11(15)

InchiKey: JHRWXGFEWCOQJC-UHFFFAOYSA-N

Formula: C14H20F8O2

SMILES: CCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 372.29

Physical Properties

Property code	Value	Unit	Source
gf	-1719.32	kJ/mol	Joback Method
hf	-2177.50	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	45.10	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.451		Crippen Method
mcvol	229.720	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
tb	580.04	K	Joback Method
tc	726.86	K	Joback Method
tf	316.68	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.89	J/mol×K	580.04	Joback Method
cpg	654.58	J/mol×K	604.51	Joback Method
cpg	668.53	J/mol×K	628.98	Joback Method
cpg	681.76	J/mol×K	653.45	Joback Method
cpg	694.32	J/mol×K	677.92	Joback Method
cpg	706.22	J/mol×K	702.39	Joback Method
cpg	717.50	J/mol×K	726.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360662&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume