Hexanoic acid, 3,5,5-trimethyl-, 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C12H20F4O2/c1-8(6-11(2,3)4)5-9(17)18-7-12(15,16)10(13)14/h8,10H,5-7H2,1

InchiKey: NSRCNLBPDSLHSI-UHFFFAOYSA-N

Formula: C12H20F4O2

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

Mol. weight [g/mol]: 272.28

Physical Properties

Property code	Value	Unit	Source
gf	-962.20	kJ/mol	Joback Method
hf	-1348.31	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	44.83	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.892		Crippen Method
mcvol	194.460	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	539.99	K	Joback Method
tc	704.37	K	Joback Method
tf	274.36	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.96	J/mol×K	539.99	Joback Method
cpg	518.42	J/mol×K	567.39	Joback Method
cpg	533.11	J/mol×K	594.78	Joback Method
cpg	547.04	J/mol×K	622.18	Joback Method
cpg	560.26	J/mol×K	649.58	Joback Method
cpg	572.78	J/mol×K	676.97	Joback Method
cpg	584.64	J/mol×K	704.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406817&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