Hexanoic acid, 3,5,5-trimethyl-, 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C12H21F3O2/c1-8(7-11(3,4)5)6-10(16)17-9(2)12(13,14)15/h8-9H,6-7H2,1-5H3

InchiKey: UPNCIIDAFFWSOK-UHFFFAOYSA-N

Formula: C12H21F3O2

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

Mol. weight [g/mol]: 254.29

Physical Properties

Property code	Value	Unit	Source
gf	-767.39	kJ/mol	Joback Method
hf	-1152.20	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.943		Crippen Method
mcvol	192.690	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
tb	540.72	K	Joback Method
tc	712.17	K	Joback Method
tf	273.77	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.83	J/mol×K	540.72	Joback Method
cpg	510.95	J/mol×K	569.30	Joback Method
cpg	526.24	J/mol×K	597.87	Joback Method
cpg	540.74	J/mol×K	626.45	Joback Method
cpg	554.46	J/mol×K	655.02	Joback Method
cpg	567.44	J/mol×K	683.60	Joback Method
cpg	579.72	J/mol×K	712.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406816&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