Dimethylmalonic acid, hexyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C14H21F5O4/c1-4-5-6-7-8-22-10(20)12(2,3)11(21)23-9-13(15,16)14(17,18)19/

InchiKey: AZTHLVVRMUOAKF-UHFFFAOYSA-N

Formula: C14H21F5O4

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

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-1366.37	kJ/mol	Joback Method
hf	-1828.69	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	57.10	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.877		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1340.00		NIST Webbook
tb	658.96	K	Joback Method
tc	827.05	K	Joback Method
tf	402.07	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.77	J/mol×K	658.96	Joback Method
cpg	684.03	J/mol×K	686.98	Joback Method
cpg	697.47	J/mol×K	714.99	Joback Method
cpg	710.13	J/mol×K	743.01	Joback Method
cpg	722.06	J/mol×K	771.02	Joback Method
cpg	733.29	J/mol×K	799.04	Joback Method
cpg	743.84	J/mol×K	827.05	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=U361940&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume