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

Inchi: InChI=1S/C14H22F4O4/c1-4-5-6-7-8-21-11(19)13(2,3)12(20)22-9-14(17,18)10(15)16/h1

InchiKey: MIOLBVYLUHPWGC-UHFFFAOYSA-N

Formula: C14H22F4O4

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

Mol. weight [g/mol]: 330.32

Physical Properties

Property code	Value	Unit	Source
gf	-1176.84	kJ/mol	Joback Method
hf	-1629.11	kJ/mol	Joback Method
hfus	31.56	kJ/mol	Joback Method
hvap	58.82	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.580		Crippen Method
mcvol	230.080	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	662.48	K	Joback Method
tc	831.89	K	Joback Method
tf	384.06	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.58	J/mol×K	662.48	Joback Method
cpg	674.16	J/mol×K	690.71	Joback Method
cpg	687.96	J/mol×K	718.95	Joback Method
cpg	701.00	J/mol×K	747.18	Joback Method
cpg	713.31	J/mol×K	775.42	Joback Method
cpg	724.93	J/mol×K	803.65	Joback Method
cpg	735.86	J/mol×K	831.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361917&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

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