Dimethylmalonic acid, 2,2,3,4,4,4-hexafluorobutyl isobutyl ester

Inchi: InChI=1S/C13H18F6O4/c1-7(2)5-22-9(20)11(3,4)10(21)23-6-12(15,16)8(14)13(17,18)19/

InchiKey: MJRORVZCBKDAGS-UHFFFAOYSA-N

Formula: C13H18F6O4

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

Mol. weight [g/mol]: 352.27

Physical Properties

Property code	Value	Unit	Source
gf	-1574.48	kJ/mol	Joback Method
hf	-2014.72	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.291		Crippen Method
mcvol	219.530	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1225.00		NIST Webbook
tb	634.47	K	Joback Method
tc	801.64	K	Joback Method
tf	361.39	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.83	J/mol×K	634.47	Joback Method
cpg	639.63	J/mol×K	662.33	Joback Method
cpg	652.63	J/mol×K	690.19	Joback Method
cpg	664.86	J/mol×K	718.06	Joback Method
cpg	676.35	J/mol×K	745.92	Joback Method
cpg	687.14	J/mol×K	773.78	Joback Method
cpg	697.26	J/mol×K	801.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361988&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