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

Inchi: InChI=1S/C15H22F6O4/c1-9(2)6-5-7-24-11(22)13(3,4)12(23)25-8-14(17,18)10(16)15(19

InchiKey: FBHBTURQMRQIRJ-UHFFFAOYSA-N

Formula: C15H22F6O4

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

Mol. weight [g/mol]: 380.32

Physical Properties

Property code	Value	Unit	Source
gf	-1557.64	kJ/mol	Joback Method
hf	-2056.00	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.071		Crippen Method
mcvol	247.710	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	1411.00		NIST Webbook
tb	680.23	K	Joback Method
tc	848.09	K	Joback Method
tf	383.93	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.65	J/mol×K	680.23	Joback Method
cpg	747.25	J/mol×K	708.21	Joback Method
cpg	761.01	J/mol×K	736.18	Joback Method
cpg	773.95	J/mol×K	764.16	Joback Method
cpg	786.13	J/mol×K	792.14	Joback Method
cpg	797.57	J/mol×K	820.12	Joback Method
cpg	808.31	J/mol×K	848.09	Joback Method

Sources

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=U361990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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