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

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

InchiKey: MSIQMCXQQZLSDF-UHFFFAOYSA-N

Formula: C13H18F6O4

SMILES: CCCCOC(=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	-1572.04	kJ/mol	Joback Method
hf	-2009.44	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.435		Crippen Method
mcvol	219.530	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
tb	634.91	K	Joback Method
tc	799.90	K	Joback Method
tf	376.39	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.39	J/mol×K	634.91	Joback Method
cpg	638.98	J/mol×K	662.41	Joback Method
cpg	651.79	J/mol×K	689.91	Joback Method
cpg	663.85	J/mol×K	717.41	Joback Method
cpg	675.20	J/mol×K	744.91	Joback Method
cpg	685.87	J/mol×K	772.41	Joback Method
cpg	695.89	J/mol×K	799.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361989&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