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

Inchi: InChI=1S/C12H17F5O4/c1-7(2)5-20-8(18)10(3,4)9(19)21-6-11(13,14)12(15,16)17/h7H,5-

InchiKey: XESDDKQNVZVJBZ-UHFFFAOYSA-N

Formula: C12H17F5O4

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

Mol. weight [g/mol]: 320.25

Physical Properties

Property code	Value	Unit	Source
gf	-1385.65	kJ/mol	Joback Method
hf	-1792.69	kJ/mol	Joback Method
hfus	22.04	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.953		Crippen Method
mcvol	203.670	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
tb	612.76	K	Joback Method
tc	783.63	K	Joback Method
tf	364.53	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.80	J/mol×K	612.76	Joback Method
cpg	579.43	J/mol×K	641.24	Joback Method
cpg	592.26	J/mol×K	669.72	Joback Method
cpg	604.32	J/mol×K	698.20	Joback Method
cpg	615.65	J/mol×K	726.67	Joback Method
cpg	626.28	J/mol×K	755.15	Joback Method
cpg	636.24	J/mol×K	783.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361936&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