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

Inchi: InChI=1S/C12H17F5O4/c1-4-5-6-20-8(18)10(2,3)9(19)21-7-11(13,14)12(15,16)17/h4-7H

InchiKey: VSTSXMFADCPCLA-UHFFFAOYSA-N

Formula: C12H17F5O4

SMILES: CCCCOC(=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	-1383.21	kJ/mol	Joback Method
hf	-1787.41	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.097		Crippen Method
mcvol	203.670	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
tb	613.20	K	Joback Method
tc	781.52	K	Joback Method
tf	379.53	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.39	J/mol×K	613.20	Joback Method
cpg	578.77	J/mol×K	641.25	Joback Method
cpg	591.39	J/mol×K	669.31	Joback Method
cpg	603.26	J/mol×K	697.36	Joback Method
cpg	614.43	J/mol×K	725.42	Joback Method
cpg	624.92	J/mol×K	753.47	Joback Method
cpg	634.77	J/mol×K	781.52	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=U361937&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