Dimethylmalonic acid, pentyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H20F4O4/c1-4-5-6-7-20-10(18)12(2,3)11(19)21-8-13(16,17)9(14)15/h9H,4

InchiKey: BFTDUTPJQMPLME-UHFFFAOYSA-N

Formula: C13H20F4O4

SMILES: CCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1185.26	kJ/mol	Joback Method
hf	-1608.47	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.190		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
tb	639.60	K	Joback Method
tc	809.01	K	Joback Method
tf	372.79	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.46	J/mol×K	639.60	Joback Method
cpg	620.58	J/mol×K	667.84	Joback Method
cpg	633.96	J/mol×K	696.07	Joback Method
cpg	646.60	J/mol×K	724.31	Joback Method
cpg	658.55	J/mol×K	752.54	Joback Method
cpg	669.81	J/mol×K	780.78	Joback Method
cpg	680.41	J/mol×K	809.01	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=U361915&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