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

Inchi: InChI=1S/C20H33F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-28-16(26)18(2,3)17(27)29-15-19

InchiKey: ZPHDXQYRMXXVLC-UHFFFAOYSA-N

Formula: C20H33F5O4

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

Mol. weight [g/mol]: 432.47

Physical Properties

Property code	Value	Unit	Source
gf	-1315.85	kJ/mol	Joback Method
hf	-1952.53	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.218		Crippen Method
mcvol	316.390	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	796.24	K	Joback Method
tc	975.77	K	Joback Method
tf	469.69	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.70	J/mol×K	796.24	Joback Method
cpg	1026.45	J/mol×K	826.16	Joback Method
cpg	1042.21	J/mol×K	856.08	Joback Method
cpg	1057.04	J/mol×K	886.01	Joback Method
cpg	1070.99	J/mol×K	915.93	Joback Method
cpg	1084.11	J/mol×K	945.85	Joback Method
cpg	1096.46	J/mol×K	975.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361945&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