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

Inchi: InChI=1S/C24H41F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-32-20(30)22(2,3)21
InchiKey: LZMLCYGRVWAEMB-UHFFFAOYSA-N
Formula: C24H41F5O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]: 488.57

Physical Properties

Property code	Value	Unit	Source
gf	-1282.17	kJ/mol	Joback Method
hf	-2035.09	kJ/mol	Joback Method
hfus	56.65	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.778		Crippen Method
mcvol	372.750	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	887.76	K	Joback Method
tc	1089.87	K	Joback Method
tf	514.77	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.40	J/mol×K	887.76	Joback Method
cpg	1272.47	J/mol×K	921.44	Joback Method
cpg	1290.30	J/mol×K	955.13	Joback Method
cpg	1307.00	J/mol×K	988.81	Joback Method
cpg	1322.65	J/mol×K	1022.50	Joback Method
cpg	1337.34	J/mol×K	1056.18	Joback Method
cpg	1351.16	J/mol×K	1089.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361948&Units=SI

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