Dimethylmalonic acid, pentafluorophenyl undecyl ester

Inchi: InChI=1S/C22H29F5O4/c1-4-5-6-7-8-9-10-11-12-13-30-20(28)22(2,3)21(29)31-19-17(26
InchiKey: HAPKMEFZEREQOS-UHFFFAOYSA-N
Formula: C22H29F5O4
SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 452.46

Physical Properties

Property code	Value	Unit	Source
gf	-1240.43	kJ/mol	Joback Method
hf	-1797.13	kJ/mol	Joback Method
hfus	58.39	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.388		Crippen Method
mcvol	320.810	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	900.04	K	Joback Method
tc	1101.96	K	Joback Method
tf	576.41	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.98	J/mol×K	900.04	Joback Method
cpg	1046.09	J/mol×K	933.69	Joback Method
cpg	1060.03	J/mol×K	967.35	Joback Method
cpg	1072.82	J/mol×K	1001.00	Joback Method
cpg	1084.51	J/mol×K	1034.65	Joback Method
cpg	1095.10	J/mol×K	1068.30	Joback Method
cpg	1104.64	J/mol×K	1101.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363668&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

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