Dimethylmalonic acid, octyl pentafluorophenyl ester

Inchi: InChI=1S/C19H23F5O4/c1-4-5-6-7-8-9-10-27-17(25)19(2,3)18(26)28-16-14(23)12(21)11
InchiKey: HYLMLHAPCAKDFU-UHFFFAOYSA-N
Formula: C19H23F5O4
SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-1265.69	kJ/mol	Joback Method
hf	-1735.21	kJ/mol	Joback Method
hfus	50.62	kJ/mol	Joback Method
hvap	76.41	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.217		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	831.40	K	Joback Method
tc	1021.03	K	Joback Method
tf	542.60	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.49	J/mol×K	831.40	Joback Method
cpg	868.34	J/mol×K	863.00	Joback Method
cpg	881.25	J/mol×K	894.61	Joback Method
cpg	893.23	J/mol×K	926.21	Joback Method
cpg	904.30	J/mol×K	957.82	Joback Method
cpg	914.48	J/mol×K	989.42	Joback Method
cpg	923.78	J/mol×K	1021.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363665&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