Dimethylmalonic acid, dodecyl pentafluorophenyl ester

Inchi: InChI=1S/C23H31F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-31-21(29)23(2,3)22(30)32-20-18
InchiKey: RDJAMWRLXBVZKG-UHFFFAOYSA-N
Formula: C23H31F5O4
SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 466.48

Physical Properties

Property code	Value	Unit	Source
gf	-1232.01	kJ/mol	Joback Method
hf	-1817.77	kJ/mol	Joback Method
hfus	60.98	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	6.778		Crippen Method
mcvol	334.900	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	922.92	K	Joback Method
tc	1130.80	K	Joback Method
tf	587.68	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.17	J/mol×K	922.92	Joback Method
cpg	1106.72	J/mol×K	957.57	Joback Method
cpg	1121.01	J/mol×K	992.21	Joback Method
cpg	1134.06	J/mol×K	1026.86	Joback Method
cpg	1145.92	J/mol×K	1061.51	Joback Method
cpg	1156.61	J/mol×K	1096.15	Joback Method
cpg	1166.16	J/mol×K	1130.80	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=U363669&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