Dimethylmalonic acid, pentafluorophenyl tetradecyl ester

Inchi: InChI=1S/C25H35F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-33-23(31)25(2,3)24(32)34
InchiKey: YFHXVOLSTZHXJG-UHFFFAOYSA-N
Formula: C25H35F5O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 494.54

Physical Properties

Property code	Value	Unit	Source
gf	-1215.17	kJ/mol	Joback Method
hf	-1859.05	kJ/mol	Joback Method
hfus	66.16	kJ/mol	Joback Method
hvap	89.76	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.558		Crippen Method
mcvol	363.080	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2494.00		NIST Webbook
tb	968.68	K	Joback Method
tc	1191.75	K	Joback Method
tf	610.22	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.22	J/mol×K	968.68	Joback Method
cpg	1229.73	J/mol×K	1005.86	Joback Method
cpg	1244.75	J/mol×K	1043.04	Joback Method
cpg	1258.30	J/mol×K	1080.21	Joback Method
cpg	1270.44	J/mol×K	1117.39	Joback Method
cpg	1281.23	J/mol×K	1154.57	Joback Method
cpg	1290.70	J/mol×K	1191.75	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=U363671&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