Dimethylmalonic acid, pentadecyl pentafluorophenyl ester

Inchi: InChI=1S/C26H37F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-34-24(32)26(2,3)25(33
InchiKey: PZONUAINBRROJY-UHFFFAOYSA-N
Formula: C26H37F5O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 508.56

Physical Properties

Property code	Value	Unit	Source
gf	-1206.75	kJ/mol	Joback Method
hf	-1879.69	kJ/mol	Joback Method
hfus	68.75	kJ/mol	Joback Method
hvap	91.99	kJ/mol	Joback Method
log10ws	-9.60		Crippen Method
logp	7.948		Crippen Method
mcvol	377.170	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	991.56	K	Joback Method
tc	1224.02	K	Joback Method
tf	621.49	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.97	J/mol×K	991.56	Joback Method
cpg	1292.01	J/mol×K	1030.30	Joback Method
cpg	1307.40	J/mol×K	1069.05	Joback Method
cpg	1321.19	J/mol×K	1107.79	Joback Method
cpg	1333.45	J/mol×K	1146.54	Joback Method
cpg	1344.23	J/mol×K	1185.28	Joback Method
cpg	1353.59	J/mol×K	1224.02	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=U363672&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