Dimethylmalonic acid, heptadecyl pentafluorophenyl ester

Inchi: InChI=1S/C28H41F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-36-26(34)28(2,3
InchiKey: ITAFBXZUMOKTAB-UHFFFAOYSA-N
Formula: C28H41F5O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 536.61

Physical Properties

Property code	Value	Unit	Source
gf	-1189.91	kJ/mol	Joback Method
hf	-1920.97	kJ/mol	Joback Method
hfus	73.93	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	8.728		Crippen Method
mcvol	405.350	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	1037.32	K	Joback Method
tc	1292.68	K	Joback Method
tf	644.03	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.68	J/mol×K	1037.32	Joback Method
cpg	1417.86	J/mol×K	1079.88	Joback Method
cpg	1434.03	J/mol×K	1122.44	Joback Method
cpg	1448.26	J/mol×K	1165.00	Joback Method
cpg	1460.66	J/mol×K	1207.56	Joback Method
cpg	1471.31	J/mol×K	1250.12	Joback Method
cpg	1480.30	J/mol×K	1292.68	Joback Method

Sources

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=U363674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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