Diethylmalonic acid, hexadecyl pentafluorophenyl ester

Inchi: InChI=1S/C29H43F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-37-27(35)29(5-2,

InchiKey: BWBAOSVFRPMXRN-UHFFFAOYSA-N

Formula: C29H43F5O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 550.64

Physical Properties

Property code	Value	Unit	Source
gf	-1181.49	kJ/mol	Joback Method
hf	-1941.61	kJ/mol	Joback Method
hfus	76.52	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	9.118		Crippen Method
mcvol	419.440	ml/mol	McGowan Method
pc	671.16	kPa	Joback Method
rinpol	2882.00		NIST Webbook
tb	1060.20	K	Joback Method
tc	1329.29	K	Joback Method
tf	655.30	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.56	J/mol×K	1060.20	Joback Method
cpg	1481.36	J/mol×K	1105.05	Joback Method
cpg	1497.92	J/mol×K	1149.90	Joback Method
cpg	1512.35	J/mol×K	1194.75	Joback Method
cpg	1524.76	J/mol×K	1239.59	Joback Method
cpg	1535.26	J/mol×K	1284.44	Joback Method
cpg	1543.97	J/mol×K	1329.29	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=U370223&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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