Diethylmalonic acid, octadecyl pentafluorophenyl ester

Inchi: InChI=1S/C31H47F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-39-29(37)3

InchiKey: UQNAVIVIVJUNQY-UHFFFAOYSA-N

Formula: C31H47F5O4

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

Mol. weight [g/mol]: 578.69

Physical Properties

Property code	Value	Unit	Source
gf	-1164.65	kJ/mol	Joback Method
hf	-1982.89	kJ/mol	Joback Method
hfus	81.70	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-11.69		Crippen Method
logp	9.899		Crippen Method
mcvol	447.620	ml/mol	McGowan Method
pc	609.06	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	1105.96	K	Joback Method
tc	1407.69	K	Joback Method
tf	677.84	K	Joback Method
vc	1.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1589.15	J/mol×K	1105.96	Joback Method
cpg	1609.29	J/mol×K	1156.25	Joback Method
cpg	1626.64	J/mol×K	1206.54	Joback Method
cpg	1641.38	J/mol×K	1256.83	Joback Method
cpg	1653.68	J/mol×K	1307.12	Joback Method
cpg	1663.71	J/mol×K	1357.40	Joback Method
cpg	1671.65	J/mol×K	1407.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370225&Units=SI
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

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