Diethylmalonic acid, eicosyl pentafluorophenyl ester

Inchi: InChI=1S/C33H51F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-41-3

InchiKey: XXJWKBXWRZDMKE-UHFFFAOYSA-N

Formula: C33H51F5O4

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

Mol. weight [g/mol]: 606.75

Physical Properties

Property code	Value	Unit	Source
gf	-1147.81	kJ/mol	Joback Method
hf	-2024.17	kJ/mol	Joback Method
hfus	86.88	kJ/mol	Joback Method
hvap	107.57	kJ/mol	Joback Method
log10ws	-12.53		Crippen Method
logp	10.679		Crippen Method
mcvol	475.800	ml/mol	McGowan Method
pc	555.20	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1151.72	K	Joback Method
tc	1494.03	K	Joback Method
tf	700.38	K	Joback Method
vc	1.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.65	J/mol×K	1151.72	Joback Method
cpg	1738.27	J/mol×K	1208.77	Joback Method
cpg	1756.38	J/mol×K	1265.82	Joback Method
cpg	1771.28	J/mol×K	1322.87	Joback Method
cpg	1783.24	J/mol×K	1379.93	Joback Method
cpg	1792.56	J/mol×K	1436.98	Joback Method
cpg	1799.50	J/mol×K	1494.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370226&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