Diethylmalonic acid, pentafluorophenyl tetradecyl ester

Inchi: InChI=1S/C27H39F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-35-25(33)27(5-2,6-3)26
InchiKey: QZQARCIUNWTTQM-UHFFFAOYSA-N
Formula: C27H39F5O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 522.59

Physical Properties

Property code	Value	Unit	Source
gf	-1198.33	kJ/mol	Joback Method
hf	-1900.33	kJ/mol	Joback Method
hfus	71.34	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	8.338		Crippen Method
mcvol	391.260	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		NIST Webbook
tb	1014.44	K	Joback Method
tc	1257.63	K	Joback Method
tf	632.76	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.14	J/mol×K	1014.44	Joback Method
cpg	1354.73	J/mol×K	1054.97	Joback Method
cpg	1370.51	J/mol×K	1095.50	Joback Method
cpg	1384.53	J/mol×K	1136.04	Joback Method
cpg	1396.87	J/mol×K	1176.57	Joback Method
cpg	1407.61	J/mol×K	1217.10	Joback Method
cpg	1416.81	J/mol×K	1257.63	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=U370221&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