Diethylmalonic acid, 3,4-difluorobenzyl pentadecyl ester

Inchi: InChI=1S/C29H46F2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-34-27(32)29(5-2,6-3
InchiKey: PNCDBAMOXGGVCL-UHFFFAOYSA-N
Formula: C29H46F2O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 496.67

Physical Properties

Property code	Value	Unit	Source
gf	-568.17	kJ/mol	Joback Method
hf	-1318.87	kJ/mol	Joback Method
hfus	68.45	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-9.71		Crippen Method
logp	8.449		Crippen Method
mcvol	414.130	ml/mol	McGowan Method
pc	738.42	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	1047.45	K	Joback Method
tc	1294.39	K	Joback Method
tf	615.97	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.37	J/mol×K	1047.45	Joback Method
cpg	1464.00	J/mol×K	1088.61	Joback Method
cpg	1480.84	J/mol×K	1129.76	Joback Method
cpg	1495.99	J/mol×K	1170.92	Joback Method
cpg	1509.57	J/mol×K	1212.08	Joback Method
cpg	1521.68	J/mol×K	1253.24	Joback Method
cpg	1532.43	J/mol×K	1294.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369334&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

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