Diethylmalonic acid, 3,4-difluorobenzyl heptadecyl ester

Inchi: InChI=1S/C31H50F2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-36-29(34)31(5
InchiKey: YIDHDUDPCVPBHQ-UHFFFAOYSA-N
Formula: C31H50F2O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 524.72

Physical Properties

Property code	Value	Unit	Source
gf	-551.33	kJ/mol	Joback Method
hf	-1360.15	kJ/mol	Joback Method
hfus	73.63	kJ/mol	Joback Method
hvap	103.58	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	9.229		Crippen Method
mcvol	442.310	ml/mol	McGowan Method
pc	667.01	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	1093.21	K	Joback Method
tc	1364.46	K	Joback Method
tf	638.51	K	Joback Method
vc	1.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.93	J/mol×K	1093.21	Joback Method
cpg	1592.75	J/mol×K	1138.42	Joback Method
cpg	1610.46	J/mol×K	1183.63	Joback Method
cpg	1626.20	J/mol×K	1228.83	Joback Method
cpg	1640.14	J/mol×K	1274.04	Joback Method
cpg	1652.45	J/mol×K	1319.25	Joback Method
cpg	1663.27	J/mol×K	1364.46	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=U369336&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