Diethylmalonic acid, heptadecyl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C31H49F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-37-29(35)31(5

InchiKey: FKRCPQUFMSSHME-UHFFFAOYSA-N

Formula: C31H49F3O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)cc1F

Mol. weight [g/mol]: 542.71

Physical Properties

Property code	Value	Unit	Source
gf	-755.77	kJ/mol	Joback Method
hf	-1567.73	kJ/mol	Joback Method
hfus	76.32	kJ/mol	Joback Method
hvap	103.43	kJ/mol	Joback Method
log10ws	-10.88		Crippen Method
logp	9.368		Crippen Method
mcvol	444.080	ml/mol	McGowan Method
pc	646.80	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	1097.46	K	Joback Method
tc	1377.66	K	Joback Method
tf	651.62	K	Joback Method
vc	1.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1578.41	J/mol×K	1097.46	Joback Method
cpg	1598.32	J/mol×K	1144.16	Joback Method
cpg	1615.91	J/mol×K	1190.86	Joback Method
cpg	1631.36	J/mol×K	1237.56	Joback Method
cpg	1644.83	J/mol×K	1284.26	Joback Method
cpg	1656.49	J/mol×K	1330.96	Joback Method
cpg	1666.50	J/mol×K	1377.66	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=U369268&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