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

Inchi: InChI=1S/C32H51F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-38-30(36)3

InchiKey: AXHOPYGNZDQCEQ-UHFFFAOYSA-N

Formula: C32H51F3O4

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

Mol. weight [g/mol]: 556.74

Physical Properties

Property code	Value	Unit	Source
gf	-747.35	kJ/mol	Joback Method
hf	-1588.37	kJ/mol	Joback Method
hfus	78.91	kJ/mol	Joback Method
hvap	105.65	kJ/mol	Joback Method
log10ws	-11.29		Crippen Method
logp	9.758		Crippen Method
mcvol	458.170	ml/mol	McGowan Method
pc	616.34	kPa	Joback Method
rinpol	3175.00		NIST Webbook
tb	1120.34	K	Joback Method
tc	1416.56	K	Joback Method
tf	662.89	K	Joback Method
vc	1.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.44	J/mol×K	1120.34	Joback Method
cpg	1663.05	J/mol×K	1169.71	Joback Method
cpg	1681.11	J/mol×K	1219.08	Joback Method
cpg	1696.84	J/mol×K	1268.45	Joback Method
cpg	1710.43	J/mol×K	1317.82	Joback Method
cpg	1722.10	J/mol×K	1367.19	Joback Method
cpg	1732.03	J/mol×K	1416.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369269&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