Diethylmalonic acid, eicosyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C34H54F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-27-41-3

InchiKey: SAEOSRXMQZPHSU-UHFFFAOYSA-N

Formula: C34H54F4O4

SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 602.78

Physical Properties

Property code	Value	Unit	Source
gf	-912.85	kJ/mol	Joback Method
hf	-1823.04	kJ/mol	Joback Method
hfus	80.15	kJ/mol	Joback Method
hvap	107.33	kJ/mol	Joback Method
log10ws	-12.31		Crippen Method
logp	11.141		Crippen Method
mcvol	488.120	ml/mol	McGowan Method
pc	558.62	kPa	Joback Method
rinpol	3298.00		NIST Webbook
rinpol	3298.00		NIST Webbook
tb	1157.16	K	Joback Method
tc	1483.36	K	Joback Method
tf	675.92	K	Joback Method
vc	1.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1779.58	J/mol×K	1157.16	Joback Method
cpg	1803.07	J/mol×K	1211.53	Joback Method
cpg	1824.24	J/mol×K	1265.89	Joback Method
cpg	1843.50	J/mol×K	1320.26	Joback Method
cpg	1861.23	J/mol×K	1374.62	Joback Method
cpg	1877.83	J/mol×K	1428.99	Joback Method
cpg	1893.68	J/mol×K	1483.36	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=U370724&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