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

Inchi: InChI=1S/C25H36F4O4/c1-4-7-8-9-10-11-12-13-14-18-32-22(30)24(5-2,6-3)23(31)33-20
InchiKey: VKQBPXISHTXVEZ-UHFFFAOYSA-N
Formula: C25H36F4O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 476.54

Physical Properties

Property code	Value	Unit	Source
gf	-988.63	kJ/mol	Joback Method
hf	-1637.28	kJ/mol	Joback Method
hfus	56.83	kJ/mol	Joback Method
hvap	87.30	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.630		Crippen Method
mcvol	361.310	ml/mol	McGowan Method
pc	882.09	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	951.24	K	Joback Method
tc	1165.24	K	Joback Method
tf	574.49	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.47	J/mol×K	951.24	Joback Method
cpg	1225.00	J/mol×K	986.91	Joback Method
cpg	1240.28	J/mol×K	1022.57	Joback Method
cpg	1254.38	J/mol×K	1058.24	Joback Method
cpg	1267.39	J/mol×K	1093.91	Joback Method
cpg	1279.39	J/mol×K	1129.58	Joback Method
cpg	1290.46	J/mol×K	1165.24	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=U370716&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