Diethylmalonic acid, decyl 3-fluorophenyl ester

Inchi: InChI=1S/C23H35FO4/c1-4-7-8-9-10-11-12-13-17-27-21(25)23(5-2,6-3)22(26)28-20-16-1

InchiKey: XRPIEXBLDQKNKN-UHFFFAOYSA-N

Formula: C23H35FO4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 394.52

Physical Properties

Property code	Value	Unit	Source
gf	-414.25	kJ/mol	Joback Method
hf	-987.45	kJ/mol	Joback Method
hfus	50.22	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.221		Crippen Method
mcvol	327.820	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	905.92	K	Joback Method
tc	1111.68	K	Joback Method
tf	535.24	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.51	J/mol×K	905.92	Joback Method
cpg	1082.03	J/mol×K	940.21	Joback Method
cpg	1097.32	J/mol×K	974.51	Joback Method
cpg	1111.45	J/mol×K	1008.80	Joback Method
cpg	1124.45	J/mol×K	1043.09	Joback Method
cpg	1136.39	J/mol×K	1077.38	Joback Method
cpg	1147.30	J/mol×K	1111.68	Joback Method

Sources

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=U370202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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