Diethylmalonic acid, 3-fluorophenyl nonyl ester

Inchi: InChI=1S/C22H33FO4/c1-4-7-8-9-10-11-12-16-26-20(24)22(5-2,6-3)21(25)27-19-15-13-1

InchiKey: WYLHMUXICRJGKO-UHFFFAOYSA-N

Formula: C22H33FO4

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

Mol. weight [g/mol]: 380.49

Physical Properties

Property code	Value	Unit	Source
gf	-422.67	kJ/mol	Joback Method
hf	-966.81	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	83.70	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.831		Crippen Method
mcvol	313.730	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2349.00		NIST Webbook
tb	883.04	K	Joback Method
tc	1086.27	K	Joback Method
tf	523.97	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.03	J/mol×K	883.04	Joback Method
cpg	1021.31	J/mol×K	916.91	Joback Method
cpg	1036.40	J/mol×K	950.78	Joback Method
cpg	1050.37	J/mol×K	984.65	Joback Method
cpg	1063.26	J/mol×K	1018.52	Joback Method
cpg	1075.10	J/mol×K	1052.40	Joback Method
cpg	1085.96	J/mol×K	1086.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370201&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

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