Diethylmalonic acid, 3-fluorophenyl undecyl ester

Inchi: InChI=1S/C24H37FO4/c1-4-7-8-9-10-11-12-13-14-18-28-22(26)24(5-2,6-3)23(27)29-21-1

InchiKey: BQKJCLQGXTWJNZ-UHFFFAOYSA-N

Formula: C24H37FO4

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

Mol. weight [g/mol]: 408.55

Physical Properties

Property code	Value	Unit	Source
gf	-405.83	kJ/mol	Joback Method
hf	-1008.09	kJ/mol	Joback Method
hfus	52.81	kJ/mol	Joback Method
hvap	88.15	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.611		Crippen Method
mcvol	341.910	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	928.80	K	Joback Method
tc	1137.95	K	Joback Method
tf	546.51	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.60	J/mol×K	928.80	Joback Method
cpg	1143.38	J/mol×K	963.66	Joback Method
cpg	1158.89	J/mol×K	998.52	Joback Method
cpg	1173.18	J/mol×K	1033.38	Joback Method
cpg	1186.31	J/mol×K	1068.24	Joback Method
cpg	1198.33	J/mol×K	1103.10	Joback Method
cpg	1209.30	J/mol×K	1137.95	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=U370203&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