Diethylmalonic acid, dodecyl 3-fluorophenyl ester

Inchi: InChI=1S/C25H39FO4/c1-4-7-8-9-10-11-12-13-14-15-19-29-23(27)25(5-2,6-3)24(28)30-2
InchiKey: YXGNPKLRFUTSIE-UHFFFAOYSA-N
Formula: C25H39FO4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 422.57

Physical Properties

Property code	Value	Unit	Source
gf	-397.41	kJ/mol	Joback Method
hf	-1028.73	kJ/mol	Joback Method
hfus	55.40	kJ/mol	Joback Method
hvap	90.38	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.002		Crippen Method
mcvol	356.000	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	951.68	K	Joback Method
tc	1165.17	K	Joback Method
tf	557.78	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.25	J/mol×K	951.68	Joback Method
cpg	1205.33	J/mol×K	987.26	Joback Method
cpg	1221.07	J/mol×K	1022.84	Joback Method
cpg	1235.53	J/mol×K	1058.42	Joback Method
cpg	1248.79	J/mol×K	1094.01	Joback Method
cpg	1260.90	J/mol×K	1129.59	Joback Method
cpg	1271.93	J/mol×K	1165.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370204&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