Diethylmalonic acid, 3-fluorophenyl pentyl ester

Inchi: InChI=1S/C18H25FO4/c1-4-7-8-12-22-16(20)18(5-2,6-3)17(21)23-15-11-9-10-14(19)13-1

InchiKey: BCFPIXKAHFZDOQ-UHFFFAOYSA-N

Formula: C18H25FO4

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

Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-456.35	kJ/mol	Joback Method
hf	-884.25	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	74.80	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.271		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	1939.00		NIST Webbook
tb	791.52	K	Joback Method
tc	992.18	K	Joback Method
tf	478.89	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.38	J/mol×K	791.52	Joback Method
cpg	785.77	J/mol×K	824.96	Joback Method
cpg	800.10	J/mol×K	858.41	Joback Method
cpg	813.42	J/mol×K	891.85	Joback Method
cpg	825.77	J/mol×K	925.29	Joback Method
cpg	837.16	J/mol×K	958.73	Joback Method
cpg	847.65	J/mol×K	992.18	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=U370199&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