Diethylmalonic acid, 2-chloro-6-fluorophenyl pentyl ester

Inchi: InChI=1S/C18H24ClFO4/c1-4-7-8-12-23-16(21)18(5-2,6-3)17(22)24-15-13(19)10-9-11-14

InchiKey: JDWNGUBJBHXXPC-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-477.91	kJ/mol	Joback Method
hf	-911.46	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.924		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	833.93	K	Joback Method
tc	1039.72	K	Joback Method
tf	521.33	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.17	J/mol×K	833.93	Joback Method
cpg	810.31	J/mol×K	868.23	Joback Method
cpg	823.40	J/mol×K	902.53	Joback Method
cpg	835.48	J/mol×K	936.83	Joback Method
cpg	846.59	J/mol×K	971.13	Joback Method
cpg	856.75	J/mol×K	1005.43	Joback Method
cpg	866.00	J/mol×K	1039.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369675&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

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