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

Inchi: InChI=1S/C19H26ClFO4/c1-4-7-8-9-13-24-17(22)19(5-2,6-3)18(23)25-16-14(20)11-10-12

InchiKey: LQSDDGBKRMMZIM-UHFFFAOYSA-N

Formula: C19H26ClFO4

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

Mol. weight [g/mol]: 372.86

Physical Properties

Property code	Value	Unit	Source
gf	-469.49	kJ/mol	Joback Method
hf	-932.10	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.314		Crippen Method
mcvol	283.700	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	856.81	K	Joback Method
tc	1062.64	K	Joback Method
tf	532.60	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.75	J/mol×K	856.81	Joback Method
cpg	868.13	J/mol×K	891.12	Joback Method
cpg	881.42	J/mol×K	925.42	Joback Method
cpg	893.68	J/mol×K	959.73	Joback Method
cpg	904.94	J/mol×K	994.03	Joback Method
cpg	915.23	J/mol×K	1028.34	Joback Method
cpg	924.59	J/mol×K	1062.64	Joback Method

Sources

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=U369677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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