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

Inchi: InChI=1S/C15H18ClFO4/c1-4-15(5-2,13(18)20-6-3)14(19)21-12-10(16)8-7-9-11(12)17/h7

InchiKey: QFQJDLFNQWXJFC-UHFFFAOYSA-N

Formula: C15H18ClFO4

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

Mol. weight [g/mol]: 316.75

Physical Properties

Property code	Value	Unit	Source
gf	-503.17	kJ/mol	Joback Method
hf	-849.54	kJ/mol	Joback Method
hfus	33.31	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.754		Crippen Method
mcvol	227.340	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	765.29	K	Joback Method
tc	974.78	K	Joback Method
tf	487.52	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.81	J/mol×K	765.29	Joback Method
cpg	642.10	J/mol×K	800.21	Joback Method
cpg	654.42	J/mol×K	835.12	Joback Method
cpg	665.81	J/mol×K	870.04	Joback Method
cpg	676.30	J/mol×K	904.95	Joback Method
cpg	685.89	J/mol×K	939.87	Joback Method
cpg	694.64	J/mol×K	974.78	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=U369671&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

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