Diethylmalonic acid, 2-chloro-6-fluorophenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H28ClFO4/c1-6-10-16(13(4)5)25-18(23)20(7-2,8-3)19(24)26-17-14(21)11-9

InchiKey: CGWNMXRXOAAXQE-UHFFFAOYSA-N

Formula: C20H28ClFO4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl)C(C)C

Mol. weight [g/mol]: 386.88

Physical Properties

Property code	Value	Unit	Source
gf	-465.95	kJ/mol	Joback Method
hf	-963.30	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.559		Crippen Method
mcvol	297.790	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	878.81	K	Joback Method
tc	1088.76	K	Joback Method
tf	513.87	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.16	J/mol×K	878.81	Joback Method
cpg	927.94	J/mol×K	913.80	Joback Method
cpg	941.56	J/mol×K	948.79	Joback Method
cpg	954.05	J/mol×K	983.79	Joback Method
cpg	965.45	J/mol×K	1018.78	Joback Method
cpg	975.81	J/mol×K	1053.77	Joback Method
cpg	985.16	J/mol×K	1088.76	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=U369676&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