Dimethylmalonic acid, 2-chloro-6-fluorophenyl isohexyl ester

Inchi: InChI=1S/C17H22ClFO4/c1-11(2)7-6-10-22-15(20)17(3,4)16(21)23-14-12(18)8-5-9-13(14

InchiKey: SYRREAXTFHQWTL-UHFFFAOYSA-N

Formula: C17H22ClFO4

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

Mol. weight [g/mol]: 344.81

Physical Properties

Property code	Value	Unit	Source
gf	-488.77	kJ/mol	Joback Method
hf	-896.10	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.390		Crippen Method
mcvol	255.520	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	810.61	K	Joback Method
tc	1019.61	K	Joback Method
tf	495.06	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.00	J/mol×K	810.61	Joback Method
cpg	754.05	J/mol×K	845.44	Joback Method
cpg	767.05	J/mol×K	880.28	Joback Method
cpg	779.03	J/mol×K	915.11	Joback Method
cpg	790.02	J/mol×K	949.94	Joback Method
cpg	800.06	J/mol×K	984.78	Joback Method
cpg	809.17	J/mol×K	1019.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361956&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