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

Inchi: InChI=1S/C17H22ClFO4/c1-4-7-11-22-15(20)17(5-2,6-3)16(21)23-14-12(18)9-8-10-13(14
InchiKey: ZIQYTOPBTYYENL-UHFFFAOYSA-N
Formula: C17H22ClFO4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 344.81

Physical Properties

Property code	Value	Unit	Source
gf	-486.33	kJ/mol	Joback Method
hf	-890.82	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.534		Crippen Method
mcvol	255.520	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	2059.00		NIST Webbook
tb	811.05	K	Joback Method
tc	1017.47	K	Joback Method
tf	510.06	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.44	J/mol×K	811.05	Joback Method
cpg	753.32	J/mol×K	845.45	Joback Method
cpg	766.19	J/mol×K	879.86	Joback Method
cpg	778.08	J/mol×K	914.26	Joback Method
cpg	789.01	J/mol×K	948.67	Joback Method
cpg	799.02	J/mol×K	983.07	Joback Method
cpg	808.14	J/mol×K	1017.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369674&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