Diethylmalonic acid, monochloride, 3,4-difluorobenzyl ester

Inchi: InChI=1S/C14H15ClF2O3/c1-3-14(4-2,12(15)18)13(19)20-8-9-5-6-10(16)11(17)7-9/h5-7H

InchiKey: KSDRHKAAYKYYMG-UHFFFAOYSA-N

Formula: C14H15ClF2O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 304.72

Physical Properties

Property code	Value	Unit	Source
gf	-601.40	kJ/mol	Joback Method
hf	-892.79	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	67.71	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.580		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1743.00		NIST Webbook
tb	719.26	K	Joback Method
tc	924.92	K	Joback Method
tf	454.61	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.16	J/mol×K	719.26	Joback Method
cpg	569.83	J/mol×K	753.54	Joback Method
cpg	581.63	J/mol×K	787.81	Joback Method
cpg	592.58	J/mol×K	822.09	Joback Method
cpg	602.74	J/mol×K	856.37	Joback Method
cpg	612.14	J/mol×K	890.65	Joback Method
cpg	620.80	J/mol×K	924.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369340&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