Diethylmalonic acid, monochloride, pentafluorobenzyl ester

Inchi: InChI=1S/C14H12ClF5O3/c1-3-14(4-2,12(15)21)13(22)23-5-6-7(16)9(18)11(20)10(19)8(6

InchiKey: HYUVVJFEDWDPOO-UHFFFAOYSA-N

Formula: C14H12ClF5O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 358.69

Physical Properties

Property code	Value	Unit	Source
gf	-1214.72	kJ/mol	Joback Method
hf	-1515.53	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.997		Crippen Method
mcvol	214.460	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
tb	732.01	K	Joback Method
tc	920.30	K	Joback Method
tf	493.94	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.09	J/mol×K	732.01	Joback Method
cpg	588.01	J/mol×K	763.39	Joback Method
cpg	598.25	J/mol×K	794.77	Joback Method
cpg	607.82	J/mol×K	826.16	Joback Method
cpg	616.74	J/mol×K	857.54	Joback Method
cpg	625.02	J/mol×K	888.92	Joback Method
cpg	632.69	J/mol×K	920.30	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=U370007&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