Diethylmalonic acid, monochloride, 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C14H14ClF3O3/c1-3-14(4-2,12(15)19)13(20)21-7-8-5-9(16)11(18)10(17)6-8/h5

InchiKey: UXYNUOAVSGTKAE-UHFFFAOYSA-N

Formula: C14H14ClF3O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1cc(F)c(F)c(F)c1

Mol. weight [g/mol]: 322.71

Physical Properties

Property code	Value	Unit	Source
gf	-805.84	kJ/mol	Joback Method
hf	-1100.37	kJ/mol	Joback Method
hfus	35.30	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.719		Crippen Method
mcvol	210.920	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	723.51	K	Joback Method
tc	922.66	K	Joback Method
tf	467.72	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.86	J/mol×K	723.51	Joback Method
cpg	575.89	J/mol×K	756.70	Joback Method
cpg	587.11	J/mol×K	789.89	Joback Method
cpg	597.56	J/mol×K	823.09	Joback Method
cpg	607.28	J/mol×K	856.28	Joback Method
cpg	616.27	J/mol×K	889.47	Joback Method
cpg	624.58	J/mol×K	922.66	Joback Method

Sources

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=U369275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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