Diethylmalonic acid, monochloride, 2-(3,3-dimethyl-2,4-oxacyclopentyl)ethyl ester

Inchi: InChI=1S/C14H23ClO5/c1-5-14(6-2,11(15)16)12(17)18-8-7-10-9-19-13(3,4)20-10/h10H,5

InchiKey: KFWXYFZZFVDINY-UHFFFAOYSA-N

Formula: C14H23ClO5

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCCC1COC(C)(C)O1

Mol. weight [g/mol]: 306.78

Physical Properties

Property code	Value	Unit	Source
gf	-453.82	kJ/mol	Joback Method
hf	-922.78	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	73.57	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.643		Crippen Method
mcvol	230.250	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	748.83	K	Joback Method
tc	961.30	K	Joback Method
tf	485.67	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.13	J/mol×K	748.83	Joback Method
cpg	696.37	J/mol×K	784.24	Joback Method
cpg	711.89	J/mol×K	819.65	Joback Method
cpg	726.81	J/mol×K	855.07	Joback Method
cpg	741.25	J/mol×K	890.48	Joback Method
cpg	755.34	J/mol×K	925.89	Joback Method
cpg	769.19	J/mol×K	961.30	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=U368393&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