Diethylmalonic acid, monochloride, 1-tert-butyloxyprop-2-yl ester

Inchi: InChI=1S/C14H25ClO4/c1-7-14(8-2,11(15)16)12(17)19-10(3)9-18-13(4,5)6/h10H,7-9H2,1

InchiKey: UMZFDHWCGMNJNK-UHFFFAOYSA-N

Formula: C14H25ClO4

SMILES: CCC(CC)(C(=O)Cl)C(=O)OC(C)COC(C)(C)C

Mol. weight [g/mol]: 292.80

Physical Properties

Property code	Value	Unit	Source
gf	-409.53	kJ/mol	Joback Method
hf	-860.41	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.305		Crippen Method
mcvol	235.240	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
tb	702.83	K	Joback Method
tc	900.82	K	Joback Method
tf	411.62	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.02	J/mol×K	702.83	Joback Method
cpg	673.82	J/mol×K	735.83	Joback Method
cpg	688.64	J/mol×K	768.83	Joback Method
cpg	702.53	J/mol×K	801.83	Joback Method
cpg	715.52	J/mol×K	834.82	Joback Method
cpg	727.64	J/mol×K	867.82	Joback Method
cpg	738.95	J/mol×K	900.82	Joback Method
dvisc	0.0015102	Pa×s	411.62	Joback Method

dvisc	0.0006903	Pa×s	460.15	Joback Method
dvisc	0.0003663	Pa×s	508.69	Joback Method
dvisc	0.0002171	Pa×s	557.22	Joback Method
dvisc	0.0001399	Pa×s	605.76	Joback Method
dvisc	0.0000962	Pa×s	654.29	Joback Method
dvisc	0.0000697	Pa×s	702.83	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=U368398&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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