Diethylmalonic acid, monochloride, 5-methylhex-2-yl ester

Inchi: InChI=1S/C14H25ClO3/c1-6-14(7-2,12(15)16)13(17)18-11(5)9-8-10(3)4/h10-11H,6-9H2,

InchiKey: IVXYRARUUZBLTM-UHFFFAOYSA-N

Formula: C14H25ClO3

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

Mol. weight [g/mol]: 276.80

Physical Properties

Property code	Value	Unit	Source
gf	-309.81	kJ/mol	Joback Method
hf	-724.72	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.926		Crippen Method
mcvol	229.370	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	683.20	K	Joback Method
tc	876.66	K	Joback Method
tf	371.97	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.96	J/mol×K	683.20	Joback Method
cpg	643.93	J/mol×K	715.44	Joback Method
cpg	658.98	J/mol×K	747.69	Joback Method
cpg	673.16	J/mol×K	779.93	Joback Method
cpg	686.49	J/mol×K	812.17	Joback Method
cpg	699.00	J/mol×K	844.41	Joback Method
cpg	710.73	J/mol×K	876.66	Joback Method
dvisc	0.0028867	Pa×s	371.97	Joback Method

dvisc	0.0011755	Pa×s	423.84	Joback Method
dvisc	0.0005823	Pa×s	475.71	Joback Method
dvisc	0.0003312	Pa×s	527.59	Joback Method
dvisc	0.0002084	Pa×s	579.46	Joback Method
dvisc	0.0001415	Pa×s	631.33	Joback Method
dvisc	0.0001019	Pa×s	683.20	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=U369302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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