Diethylmalonic acid, monochloride, tetrahydrofurfuryl ester

Inchi: InChI=1S/C12H19ClO4/c1-3-12(4-2,10(13)14)11(15)17-8-9-6-5-7-16-9/h9H,3-8H2,1-2H3

InchiKey: FOCBRGCNKDVDQH-UHFFFAOYSA-N

Formula: C12H19ClO4

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCC1CCCO1

Mol. weight [g/mol]: 262.73

Physical Properties

Property code	Value	Unit	Source
gf	-371.34	kJ/mol	Joback Method
hf	-744.40	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.280		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	680.55	K	Joback Method
tc	893.93	K	Joback Method
tf	416.90	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.14	J/mol×K	680.55	Joback Method
cpg	609.70	J/mol×K	858.37	Joback Method
cpg	598.13	J/mol×K	822.81	Joback Method
cpg	585.64	J/mol×K	787.24	Joback Method
cpg	572.17	J/mol×K	751.68	Joback Method
cpg	557.69	J/mol×K	716.11	Joback Method
cpg	620.39	J/mol×K	893.93	Joback Method
dvisc	0.0001979	Pa×s	680.55	Joback Method

dvisc	0.0002577	Pa×s	636.61	Joback Method
dvisc	0.0003490	Pa×s	592.67	Joback Method
dvisc	0.0004962	Pa×s	548.73	Joback Method
dvisc	0.0007501	Pa×s	504.78	Joback Method
dvisc	0.0012268	Pa×s	460.84	Joback Method
dvisc	0.0022258	Pa×s	416.90	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=U370650&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