Diethylmalonic acid, monochloride, 4-nitrophenyl ester

Inchi: InChI=1S/C13H14ClNO5/c1-3-13(4-2,11(14)16)12(17)20-10-7-5-9(6-8-10)15(18)19/h5-8

InchiKey: YGDHCRACFJXLRA-UHFFFAOYSA-N

Formula: C13H14ClNO5

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 299.71

Physical Properties

Property code	Value	Unit	Source
gf	-175.02	kJ/mol	Joback Method
hf	-479.22	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	83.05	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.072		Crippen Method
mcvol	208.940	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2061.00		NIST Webbook
tb	844.70	K	Joback Method
tc	1088.19	K	Joback Method
tf	573.25	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.76	J/mol×K	844.70	Joback Method
cpg	595.62	J/mol×K	885.28	Joback Method
cpg	605.44	J/mol×K	925.86	Joback Method
cpg	614.30	J/mol×K	966.44	Joback Method
cpg	622.27	J/mol×K	1007.03	Joback Method
cpg	629.41	J/mol×K	1047.61	Joback Method
cpg	635.80	J/mol×K	1088.19	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=U370172&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

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