Dimethylmalonic acid, ethyl 3-nitrophenyl ester

Inchi: InChI=1S/C13H15NO6/c1-4-19-11(15)13(2,3)12(16)20-10-7-5-6-9(8-10)14(17)18/h5-8H,
InchiKey: HKGFQZNVWYAOCJ-UHFFFAOYSA-N
Formula: C13H15NO6
SMILES: CCOC(=O)C(C)(C)C(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 281.26

Physical Properties

Property code	Value	Unit	Source
gf	-268.09	kJ/mol	Joback Method
hf	-595.70	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	81.08	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.089		Crippen Method
mcvol	202.570	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	829.69	K	Joback Method
tc	1068.02	K	Joback Method
tf	565.56	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.03	J/mol×K	829.69	Joback Method
cpg	600.66	J/mol×K	869.41	Joback Method
cpg	611.16	J/mol×K	909.13	Joback Method
cpg	620.58	J/mol×K	948.86	Joback Method
cpg	628.96	J/mol×K	988.58	Joback Method
cpg	636.33	J/mol×K	1028.30	Joback Method
cpg	642.75	J/mol×K	1068.02	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=U363602&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