Dimethylmalonic acid, 3-nitrophenyl propyl ester

Inchi: InChI=1S/C14H17NO6/c1-4-8-20-12(16)14(2,3)13(17)21-11-7-5-6-10(9-11)15(18)19/h5-7

InchiKey: YCOQSTREPBLTAU-UHFFFAOYSA-N

Formula: C14H17NO6

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 295.29

Physical Properties

Property code	Value	Unit	Source
gf	-259.67	kJ/mol	Joback Method
hf	-616.34	kJ/mol	Joback Method
hfus	35.19	kJ/mol	Joback Method
hvap	83.30	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.480		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	852.57	K	Joback Method
tc	1087.40	K	Joback Method
tf	576.83	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.79	J/mol×K	852.57	Joback Method
cpg	655.68	J/mol×K	891.71	Joback Method
cpg	666.43	J/mol×K	930.85	Joback Method
cpg	676.08	J/mol×K	969.98	Joback Method
cpg	684.69	J/mol×K	1009.12	Joback Method
cpg	692.28	J/mol×K	1048.26	Joback Method
cpg	698.91	J/mol×K	1087.40	Joback Method

Sources

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=U363603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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