Dimethylmalonic acid, di(3-nitrophenyl) ester

Inchi: InChI=1S/C17H14N2O8/c1-17(2,15(20)26-13-7-3-5-11(9-13)18(22)23)16(21)27-14-8-4-6
InchiKey: HSCHZYIALMNTOP-UHFFFAOYSA-N
Formula: C17H14N2O8
SMILES: CC(C)(C(=O)Oc1cccc([N+](=O)[O-])c1)C(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 374.30

Physical Properties

Property code	Value	Unit	Source
gf	-96.08	kJ/mol	Joback Method
hf	-463.96	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	109.51	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.040		Crippen Method
mcvol	252.590	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	2925.00		NIST Webbook
tb	1104.71	K	Joback Method
tc	1380.07	K	Joback Method
tf	793.19	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.92	J/mol×K	1104.71	Joback Method
cpg	786.87	J/mol×K	1150.60	Joback Method
cpg	791.60	J/mol×K	1196.50	Joback Method
cpg	795.20	J/mol×K	1242.39	Joback Method
cpg	797.79	J/mol×K	1288.28	Joback Method
cpg	799.45	J/mol×K	1334.18	Joback Method
cpg	800.31	J/mol×K	1380.07	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=U363611&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