Dimethylmalonic acid, isobutyl 3-nitrophenyl ester

Inchi: InChI=1S/C15H19NO6/c1-10(2)9-21-13(17)15(3,4)14(18)22-12-7-5-6-11(8-12)16(19)20/h
InchiKey: HLRAZGSEIFKIRX-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
gf	-253.69	kJ/mol	Joback Method
hf	-642.26	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	85.14	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.726		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	875.01	K	Joback Method
tc	1110.26	K	Joback Method
tf	573.10	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.00	J/mol×K	875.01	Joback Method
cpg	712.24	J/mol×K	914.22	Joback Method
cpg	723.28	J/mol×K	953.43	Joback Method
cpg	733.17	J/mol×K	992.64	Joback Method
cpg	741.95	J/mol×K	1031.85	Joback Method
cpg	749.68	J/mol×K	1071.05	Joback Method
cpg	756.40	J/mol×K	1110.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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