Dimethylmalonic acid, butyl 3-nitrophenyl ester

Inchi: InChI=1S/C15H19NO6/c1-4-5-9-21-13(17)15(2,3)14(18)22-12-8-6-7-11(10-12)16(19)20/h

InchiKey: JAEPINGBINLTCR-UHFFFAOYSA-N

Formula: C15H19NO6

SMILES: CCCCOC(=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	-251.25	kJ/mol	Joback Method
hf	-636.98	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.870		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2121.00		NIST Webbook
tb	875.45	K	Joback Method
tc	1107.42	K	Joback Method
tf	588.10	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.43	J/mol×K	875.45	Joback Method
cpg	711.53	J/mol×K	914.11	Joback Method
cpg	722.48	J/mol×K	952.77	Joback Method
cpg	732.33	J/mol×K	991.44	Joback Method
cpg	741.11	J/mol×K	1030.10	Joback Method
cpg	748.88	J/mol×K	1068.76	Joback Method
cpg	755.68	J/mol×K	1107.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363605&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