Diethylmalonic acid, isobutyl 3-nitrophenyl ester

Inchi: InChI=1S/C17H23NO6/c1-5-17(6-2,15(19)23-11-12(3)4)16(20)24-14-9-7-8-13(10-14)18(

InchiKey: CKVREVCHMQOBDD-UHFFFAOYSA-N

Formula: C17H23NO6

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-236.85	kJ/mol	Joback Method
hf	-683.54	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	89.59	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.506		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	920.77	K	Joback Method
tc	1151.70	K	Joback Method
tf	595.64	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.63	J/mol×K	920.77	Joback Method
cpg	826.16	J/mol×K	959.26	Joback Method
cpg	837.46	J/mol×K	997.75	Joback Method
cpg	847.59	J/mol×K	1036.24	Joback Method
cpg	856.61	J/mol×K	1074.72	Joback Method
cpg	864.57	J/mol×K	1113.21	Joback Method
cpg	871.51	J/mol×K	1151.70	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=U370525&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