Dimethylmalonic acid, 3-nitrophenyl octyl ester

Inchi: InChI=1S/C19H27NO6/c1-4-5-6-7-8-9-13-25-17(21)19(2,3)18(22)26-16-12-10-11-15(14-1

InchiKey: HSUGNIVJFMUHOO-UHFFFAOYSA-N

Formula: C19H27NO6

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

Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-217.57	kJ/mol	Joback Method
hf	-719.54	kJ/mol	Joback Method
hfus	48.14	kJ/mol	Joback Method
hvap	94.43	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.430		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2495.00		NIST Webbook
tb	966.97	K	Joback Method
tc	1194.79	K	Joback Method
tf	633.18	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.61	J/mol×K	966.97	Joback Method
cpg	942.31	J/mol×K	1004.94	Joback Method
cpg	953.78	J/mol×K	1042.91	Joback Method
cpg	964.10	J/mol×K	1080.88	Joback Method
cpg	973.31	J/mol×K	1118.85	Joback Method
cpg	981.47	J/mol×K	1156.82	Joback Method
cpg	988.65	J/mol×K	1194.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363610&Units=SI

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