Dimethylmalonic acid, heptyl 3-nitrophenyl ester

Inchi: InChI=1S/C18H25NO6/c1-4-5-6-7-8-12-24-16(20)18(2,3)17(21)25-15-11-9-10-14(13-15)

InchiKey: HHQBNERZNBFSDE-UHFFFAOYSA-N

Formula: C18H25NO6

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

Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
gf	-225.99	kJ/mol	Joback Method
hf	-698.90	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.040		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook
tb	944.09	K	Joback Method
tc	1171.77	K	Joback Method
tf	621.91	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.04	J/mol×K	944.09	Joback Method
cpg	883.61	J/mol×K	982.04	Joback Method
cpg	894.98	J/mol×K	1019.98	Joback Method
cpg	905.20	J/mol×K	1057.93	Joback Method
cpg	914.34	J/mol×K	1095.88	Joback Method
cpg	922.43	J/mol×K	1133.82	Joback Method
cpg	929.55	J/mol×K	1171.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363609&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

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