Diethylmalonic acid, 4-nitrophenyl propyl ester

Inchi: InChI=1S/C16H21NO6/c1-4-11-22-14(18)16(5-2,6-3)15(19)23-13-9-7-12(8-10-13)17(20)

InchiKey: KSEWQNRGWVNVGQ-UHFFFAOYSA-N

Formula: C16H21NO6

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-242.83	kJ/mol	Joback Method
hf	-657.62	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.260		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2181.00		NIST Webbook
tb	898.33	K	Joback Method
tc	1128.13	K	Joback Method
tf	599.37	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.89	J/mol×K	898.33	Joback Method
cpg	768.17	J/mol×K	936.63	Joback Method
cpg	779.29	J/mol×K	974.93	Joback Method
cpg	789.28	J/mol×K	1013.23	Joback Method
cpg	798.21	J/mol×K	1051.53	Joback Method
cpg	806.12	J/mol×K	1089.83	Joback Method
cpg	813.05	J/mol×K	1128.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370161&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