Diethylmalonic acid, di(2-nitrophenyl) ester

Inchi: InChI=1S/C19H18N2O8/c1-3-19(4-2,17(22)28-15-11-7-5-9-13(15)20(24)25)18(23)29-16-12-8-6-10-14(16)21(26)27/h5-12H,3-4H2,1-2H3
InchiKey: XLYAOZWMHOFPKC-UHFFFAOYSA-N
Formula: C19H18N2O8
SMILES: CCC(CC)(C(=O)Oc1ccccc1[N+](=O)[O-])C(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 402.35

Physical Properties

Property code	Value	Unit	Source
gf	-79.24	kJ/mol	Joback Method
hf	-505.24	kJ/mol	Joback Method
hfus	53.15	kJ/mol	Joback Method
hvap	113.96	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	3.820		Crippen Method
mcvol	280.770	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2987.00		NIST Webbook
tb	1150.47	K	Joback Method
tc	1422.61	K	Joback Method
tf	815.73	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.86	J/mol×K	1150.47	Joback Method
cpg	902.04	J/mol×K	1195.83	Joback Method
cpg	907.02	J/mol×K	1241.18	Joback Method
cpg	910.93	J/mol×K	1286.54	Joback Method
cpg	913.86	J/mol×K	1331.89	Joback Method
cpg	915.94	J/mol×K	1377.25	Joback Method
cpg	917.27	J/mol×K	1422.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369863&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