Pimelic acid, di(2-nitrophenyl) ester

Inchi: InChI=1S/C19H18N2O8/c22-18(28-16-10-6-4-8-14(16)20(24)25)12-2-1-3-13-19(23)29-17
InchiKey: ZPTDXNWYBZXQCH-UHFFFAOYSA-N
Formula: C19H18N2O8
SMILES: O=C(CCCCCC(=O)Oc1ccccc1[N+](=O)[O-])Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 402.35

Physical Properties

Property code	Value	Unit	Source
gf	-82.08	kJ/mol	Joback Method
hf	-496.49	kJ/mol	Joback Method
hfus	60.57	kJ/mol	Joback Method
hvap	115.26	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	3.965		Crippen Method
mcvol	280.770	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook
tb	1153.70	K	Joback Method
tc	1420.54	K	Joback Method
tf	813.31	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.89	J/mol×K	1153.70	Joback Method
cpg	898.98	J/mol×K	1198.17	Joback Method
cpg	902.59	J/mol×K	1242.65	Joback Method
cpg	904.77	J/mol×K	1287.12	Joback Method
cpg	905.61	J/mol×K	1331.59	Joback Method
cpg	905.17	J/mol×K	1376.07	Joback Method
cpg	903.51	J/mol×K	1420.54	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=U416749&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