N,N-Dimethyl-2-(3-nitro-phenyl)-2-(3-nitro-phenyl)

Inchi: InChI=1S/C16H15N3O5/c1-17(2)16(20)15(11-5-3-7-13(9-11)18(21)22)12-6-4-8-14(10-12
InchiKey: MTNYNHVOPZEMIO-UHFFFAOYSA-N
Formula: C16H15N3O5
SMILES: CN(C)C(=O)C(c1cccc([N+](=O)[O-])c1)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 329.31

Physical Properties

Property code	Value	Unit	Source
gf	339.92	kJ/mol	Joback Method
hf	4.70	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	2.723		Crippen Method
mcvol	235.170	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	998.35	K	Joback Method
tc	1268.64	K	Joback Method
tf	702.58	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.31	J/mol×K	998.35	Joback Method
cpg	731.32	J/mol×K	1043.40	Joback Method
cpg	740.29	J/mol×K	1088.45	Joback Method
cpg	748.38	J/mol×K	1133.49	Joback Method
cpg	755.71	J/mol×K	1178.54	Joback Method
cpg	762.42	J/mol×K	1223.59	Joback Method
cpg	768.65	J/mol×K	1268.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R277835&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

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