N'-(2,4-dinitrophenyl)-n,n-dimethylurea

Inchi: InChI=1S/C9H10N4O5/c1-11(2)9(14)10-7-4-3-6(12(15)16)5-8(7)13(17)18/h3-5H,1-2H3,(
InchiKey: YNGYYVJAOOEVDA-UHFFFAOYSA-N
Formula: C9H10N4O5
SMILES: CN(C)C(=O)Nc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 254.20
CAS: 73953-80-7

Physical Properties

Property code	Value	Unit	Source
gf	260.40	kJ/mol	Joback Method
hf	-28.60	kJ/mol	Joback Method
hfus	44.77	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	1.596		Crippen Method
mcvol	170.280	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	862.12	K	Joback Method
tc	1118.79	K	Joback Method
tf	664.93	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.30	J/mol×K	862.12	Joback Method
cpg	498.41	J/mol×K	904.90	Joback Method
cpg	506.60	J/mol×K	947.68	Joback Method
cpg	513.92	J/mol×K	990.46	Joback Method
cpg	520.45	J/mol×K	1033.23	Joback Method
cpg	526.25	J/mol×K	1076.01	Joback Method
cpg	531.41	J/mol×K	1118.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73953807&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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