

2,4-Dinitro-1,3-dimethyl-benzene

Other names:	2,4-Dinitro-m-xylene Benzene, 1,3-dimethyl-2,4-dinitro- m-Xylene, 2,4-dinitro-
Inchi:	InChI=1S/C8H8N2O4/c1-5-3-4-7(9(11)12)6(2)8(5)10(13)14/h3-4H,1-2H3
InchiKey:	XUUSVHGZGPBZLS-UHFFFAOYSA-N
Formula:	C8H8N2O4
SMILES:	<chem>Cc1ccc([N+](=O)[O-])c(C)c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	196.16
CAS:	603-02-1

Physical Properties

Property code	Value	Unit	Source
chs	-4205.80 ± 4.20	kJ/mol	NIST Webbook
gf	171.10	kJ/mol	Joback Method
hf	-27.85	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.120		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	727.74	K	Joback Method
tc	995.84	K	Joback Method
tf	531.12	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/molxK	727.74	Joback Method
cpg	356.93	J/molxK	772.42	Joback Method
cpg	366.45	J/molxK	817.11	Joback Method
cpg	375.11	J/molxK	861.79	Joback Method
cpg	382.95	J/molxK	906.47	Joback Method

cpg	390.01	J/mol×K	951.16	Joback Method
cpg	396.32	J/mol×K	995.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C603021&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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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