

Benzene, 1,3,5-trimethyl-2,4-dinitro-

Other names:	Mesitylene, 2,4-dinitro- Dinitromesitylene 2,4-Dinitromesitylene 2,4-Dinitro-1,3,5-trimethylbenzene
Inchi:	InChI=1S/C9H10N2O4/c1-5-4-6(2)9(11(14)15)7(3)8(5)10(12)13/h4H,1-3H3
InchiKey:	OFMLQCPPVSVIDD-UHFFFAOYSA-N
Formula:	C9H10N2O4
SMILES:	<chem>Cc1cc(C)c([N+](=O)[O-])c(C)c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	210.19
CAS:	608-50-4

Physical Properties

Property code	Value	Unit	Source
gf	169.89	kJ/mol	Joback Method
hf	-59.96	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.428		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	755.60	K	Joback Method
tc	1018.02	K	Joback Method
tf	358.00 ± 2.00	K	NIST Webbook
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.95	J/molxK	755.60	Joback Method
cpg	405.99	J/molxK	799.34	Joback Method
cpg	416.12	J/molxK	843.07	Joback Method
cpg	425.36	J/molxK	886.81	Joback Method
cpg	433.76	J/molxK	930.55	Joback Method

cpg	441.34	J/mol×K	974.29	Joback Method
cpg	448.12	J/mol×K	1018.02	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=C608504&Units=SI

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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