2,4-DINITRO-M-XYLENE

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: Cc1ccc([N+](=O)[O-])c(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 196.16

Physical Properties

Property code	Value	Unit	Source
chs	-4205.80 ± 4.20	kJ/mol	NIST Webbook
hf	13.63	kJ/mol	Cheméo Relay (1.0)
hfus	32.07	kJ/mol	Joback Method
hvap	77.63	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-3.36		Cheméo Relay (1.0)
logp	2.120		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
tb	544.64	K	Cheméo Relay (1.0)
tf	337.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.56	J/mol×K	727.94	Joback Method
cpg	356.98	J/mol×K	772.64	Joback Method
cpg	366.50	J/mol×K	817.33	Joback Method
cpg	375.16	J/mol×K	862.03	Joback Method
cpg	382.99	J/mol×K	906.72	Joback Method
cpg	390.04	J/mol×K	951.42	Joback Method
cpg	396.35	J/mol×K	996.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603021&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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