

2,4,6-Trinitro-N-(methylnitro)-m-toluidine

Inchi: InChI=1S/C8H7N5O8/c1-4-5(10(14)15)3-6(11(16)17)8(7(4)12(18)19)9(2)13(20)21/h3H,1
InchiKey: OUUSHEOSJOFZTA-UHFFFAOYSA-N
Formula: C8H7N5O8
SMILES: Cc1c([N+](=O)[O-])cc([N+](=O)[O-])c(N(C)[N+](=O)[O-])c1[N+](=O)[O-]
Mol. weight [g/mol]: 301.17
CAS: 43072-20-4

Physical Properties

Property code	Value	Unit	Source
chs	-4160.00 ± 3.00	kJ/mol	NIST Webbook
gf	343.35	kJ/mol	Joback Method
hf	6.69	kJ/mol	Joback Method
hfs	10.00 ± 3.00	kJ/mol	NIST Webbook
hfus	57.43	kJ/mol	Joback Method
hvap	106.73	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	1.348		Crippen Method
mcvol	179.480	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	1048.84	K	Joback Method
tc	1338.91	K	Joback Method
tf	375.60 ± 0.20	K	NIST Webbook
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.96	J/mol×K	1048.84	Joback Method
cpg	536.59	J/mol×K	1097.18	Joback Method
cpg	541.35	J/mol×K	1145.53	Joback Method
cpg	545.33	J/mol×K	1193.87	Joback Method
cpg	548.63	J/mol×K	1242.22	Joback Method
cpg	551.32	J/mol×K	1290.56	Joback Method
cpg	553.49	J/mol×K	1338.91	Joback Method

cps	326.40	J/mol×K	298.00	NIST Webbook
hfust	19.33	kJ/mol	375.60	NIST Webbook
hfust	19.33	kJ/mol	375.60	NIST Webbook
sfust	51.50	J/mol×K	375.60	NIST Webbook

Sources

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=C43072204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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