5-tert-Butyl-4,6-dinitro-1,2,3-trimethylbenzene

Other names:	Benzene, 1-(1,1-dimethylethyl)-3,4,5-trimethyl-2,6-dinitro-
	Benzene, 1-(1,1-dimethylethyl)-2,6-dinitro-3,4,5-trimethyl-
	Benzene, 1-tert-butyl-2,6-dinitro-3,4,5-trimethyl-
	Benzene, 1-tert-butyl-3,4,5-trimethyl-2,6-dinitro-
	Musk tibetene
	Tibetene musk
	5-tert-Butyl-1,2,3-trimethyl-4,6-dinitrobenzene
	5-t-Butyl-4,6-dinitro-1,2,3-trimethylbenzene
	Musk tibetine
	NSC 78470
	1-tert-Butyl-2,6-dinitro-3,4,5-trimethylbenzene
	1-tert-butyl-3,4,5-trimethyl-2,6-dinitrobenzene
Inchi:	InChI=1S/C13H18N2O4/c1-7-8(2)11(14(16)17)10(13(4,5)6)12(9(7)3)15(18)19/h1-6H3
InchiKey:	MINYPECWDZURGR-UHFFFAOYSA-N
Formula:	C13H18N2O4
SMILES:	Cc1c(C)c([N+](=O)[O-])c(C(C)(C)C)c([N+](=O)[O-])c1C
Mol. weight [g/mol]:	266.29
CAS:	145-39-1

Physical Properties

Property code	Value	Unit	Source
gf	196.78	kJ/mol	Joback Method
hf	-162.74	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.726		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1907.30		NIST Webbook
tb	848.87	K	Joback Method
tc	1103.46	K	Joback Method
tf	614.93	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.06	J/mol×K	848.87	Joback Method
cpg	621.19	J/mol×K	891.30	Joback Method
cpg	633.27	J/mol×K	933.73	Joback Method
cpg	644.37	J/mol×K	976.16	Joback Method
cpg	654.57	J/mol×K	1018.59	Joback Method
cpg	663.94	J/mol×K	1061.03	Joback Method
cpg	672.54	J/mol×K	1103.46	Joback Method

Sources

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=C145391&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume