Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro-

Other names: 1-tert-Butyl-3,5-dimethyl-2,4,6-trinitrobenzene
2,4,6-Trinitro-1,3-dimethyl-5-t-butylbenzene
2,4,6-Trinitro-1,3-dimethyl-5-tert-butylbenzene
2,4,6-Trinitro-5-tert-butyl-m-xylene
2,4,6-trinitro-3,5-dimethyl-tert-butylbenzene
5-t-Butyl-2,4,6-trinitro-m-xylene
5-tert-Butyl-2,4,6-trinitro-m-xylene
5-tert-Butyl-2,4,6-trinitroxylene
Benzene, 1-tert-butyl-3,5-dimethyl-2,4,6-trinitro-
Musk xylene
Musk xylol
NSC 59844
m-xylene, 5-tert-butyl-2,4,6-trinitro-
xylene musk

Inchi: InChI=1S/C12H15N3O6/c1-6-9(13(16)17)7(2)11(15(20)21)8(12(3,4)5)10(6)14(18)19/h1-5

InchiKey: XMWRWTSZNLOZFN-UHFFFAOYSA-N

Formula: C12H15N3O6

SMILES: Cc1c([N+](=O)[O-])c(C)c([N+](=O)[O-])c(C(C)(C)C)c1[N+](=O)[O-]

Mol. weight [g/mol]: 297.26

CAS: 81-15-2

Physical Properties

Property code	Value	Unit	Source
gf	223.91	kJ/mol	Joback Method
hf	-152.86	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	96.37	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	3.326		Crippen Method
mcvol	208.440	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1813.60		NIST Webbook
rinpol	1813.60		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1813.60		NIST Webbook
tb	977.83	K	Joback Method

tc	1251.52	K	Joback Method
tf	747.27	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.47	J/mol×K	1160.29	Joback Method
cpg	681.20	J/mol×K	1205.91	Joback Method
cpg	639.87	J/mol×K	977.83	Joback Method
cpg	649.86	J/mol×K	1023.45	Joback Method
cpg	658.89	J/mol×K	1069.06	Joback Method
cpg	667.06	J/mol×K	1114.68	Joback Method
cpg	687.36	J/mol×K	1251.52	Joback Method
hfust	20.79	kJ/mol	386.70	NIST Webbook
hsubt	100.40	kJ/mol	330.00	NIST Webbook

Sources

Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
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=C81152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and correlation of solubility and solution thermodynamics of musk xylene in different pure solvents:	https://www.doi.org/10.1016/j.jct.2019.03.029

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume