Musk ketone

Other names:	1-(4-(tert-butyl)-2,6-dimethyl-3,5-dinitrophenyl)ethan-1-one
	1-Acetyl-4-tert-butyl-2,6-dimethyl-3,5-dinitrobenzene
	1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]ethanone
	2,6-Dimethyl-3,5-dinitro-4-t-butylacetophenone
	2,6-Dimethyl-3,5-dinitro-4-tert-butylacetophenone
	2,6-Dinitro-3,5-dimethyl-4-acetyl-tertbutylbenzene
	3',5'-dinitro-2',6'-dimethyl-4'-tert-butylacetophenone
	3,5-Dinitro-2,6-dimethyl-4-tert-butyl acetophenone
	4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone
	4-t-Butyl-2,6-dimethyl-3,5-dinitroacetophenone
	4-tert-Butyl-2,6-dimethyl-3,5-dinitroacetophenone
	4-tert-Butyl-2,6-dimethyl-3,5-dinitroactophenone
	4-tert-Butyl-3,5-dinitro-2,6-dimethylacetophenone
	Acetophenone, 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitro-
	Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-
	Ketone Moschus
	Ketone musk
	NSC 15339
Inchi:	InChI=1S/C14H18N2O5/c1-7-10(9(3)17)8(2)13(16(20)21)11(14(4,5)6)12(7)15(18)19/h1-6
InchiKey:	WXCMHFPAUCOJIG-UHFFFAOYSA-N
Formula:	C14H18N2O5
SMILES:	CC(=O)c1c(C)c([N+](=O)[O-])c(C(C)(C)C)c([N+](=O)[O-])c1C
Mol. weight [g/mol]:	294.30
CAS:	81-14-1

Physical Properties

Property code	Value	Unit	Source
gf	76.28	kJ/mol	Joback Method
hf	-295.96	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	3.620		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1942.80		NIST Webbook
rinpol	1922.20		NIST Webbook

rinpol	1925.00		NIST Webbook
rinpol	1942.80		NIST Webbook
tb	925.62	K	Joback Method
tc	1180.03	K	Joback Method
tf	676.13	K	Joback Method
tt	409.50	K	Determination and Correlation of the Solubility of Musk Ketone in Pure and Binary Solvents at 273.15-313.15 K
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.70	J/mol×K	1095.22	Joback Method
cpg	719.65	J/mol×K	1137.63	Joback Method
cpg	671.19	J/mol×K	925.62	Joback Method
cpg	682.76	J/mol×K	968.02	Joback Method
cpg	693.33	J/mol×K	1010.42	Joback Method
cpg	702.95	J/mol×K	1052.82	Joback Method
cpg	726.88	J/mol×K	1180.03	Joback Method
hfust	23.81	kJ/mol	408.50	NIST Webbook
hsubt	107.90	kJ/mol	323.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Correlation of the Solubility of Musk Ketone in Pure and Binary Solvents at 273.15-313.15 K:	https://www.doi.org/10.1021/acs.jced.9b00310
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=C81141&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
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
tt:	Triple Point Temperature
vc:	Critical Volume