Musk ambrette (artificial)

Other names:	Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro-
	Anisole, 6-tert-butyl-3-methyl-2,4-dinitro-
	Amber musk
	Musk ambrette
	Synthetic musk ambrette
	6-tert-Butyl-3-Methyl-2,4-dinitroanisol
	2-tert-Butyl-4,6-dinitro-5-methylanisole
	2,4-Dinitro-3-methyl-6-tert-butylanisole
	4-tert-Butyl-2,6-dinitro-3-methoxytoluene
	6-tert-Butyl-3-methyl-2,4-dinitroanisole
	2,6-Dinitro-3-methoxy-4-tert-butyltoluene
	Anisole, 6-t-butyl-3-methyl-2,4-dinitro-
	Artificial musk ambrette
	1-(1,1-Dimethylethyl)-2-methoxy-4-methyl-3,5-dinitrobenzene
	1-Methyl-4-t-butyl-3-methoxy-2,6-dinitrobenzene
	5-t-Butyl-1,3-dinitro-4-methoxy-2-methylbenzene
	6-t-Butyl-3-methyl-2,4-dinitroanisole
	Musk amberette
	4-tert-Butyl-3-methoxy-2,6-dinitrotoluene
	Ambrette musk
	NSC 46122
	1-Methyl-4-tert-butyl-3-methoxy-2,6-dinitrobenzene
Inchi:	InChI=1S/C12H16N2O5/c1-7-9(13(15)16)6-8(12(2,3)4)11(19-5)10(7)14(17)18/h6H,1-5H3
InchiKey:	SUAUILGSCPYJCS-UHFFFAOYSA-N
Formula:	C12H16N2O5
SMILES:	COc1c(C(C)(C)C)cc([N+](=O)[O-])c(C)c1[N+](=O)[O-]
Mol. weight [g/mol]:	268.27
CAS:	83-66-9

Physical Properties

Property code	Value	Unit	Source
gf	92.99	kJ/mol	Joback Method
hf	-262.85	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method

logp	3.118		Crippen Method
mcvol	196.890	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
tb	843.43	K	Joback Method
tc	1098.52	K	Joback Method
tf	613.37	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	843.43	Joback Method
cpg	592.38	J/mol×K	885.94	Joback Method
cpg	603.61	J/mol×K	928.46	Joback Method
cpg	613.79	J/mol×K	970.97	Joback Method
cpg	622.97	J/mol×K	1013.49	Joback Method
cpg	631.20	J/mol×K	1056.00	Joback Method
cpg	638.53	J/mol×K	1098.52	Joback Method
hsubt	102.90	kJ/mol	323.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C83669&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume