4,6-Dinitro-1,1,3,3,5-pentamethylindane

Other names:	1H-Indene, 2,3-dihydro-1,1,3,3,5-pentamethyl-4,6-dinitro- Indan, 1,1,3,3,5-pentamethyl-4,6-dinitro- Moskene 1,1,3,3,5-Pentamethyl-4,6-dinitroindan 1,1,3,3,5-Pentamethyl-4,6-dinitrolindan Indan, 4,6-dinitro-1,1,3,3,5-pentamethyl- 1,1,3,3,5-Pentamethyl-4,6-dinitroindane Musk moskene
Inchi:	InChI=1S/C14H18N2O4/c1-8-10(15(17)18)6-9-11(12(8)16(19)20)14(4,5)7-13(9,2)3/h6H,1
InchiKey:	UHWURQRPEIFIAK-UHFFFAOYSA-N
Formula:	C14H18N2O4
SMILES:	Cc1c([N+](=O)[O-])cc2c(c1[N+](=O)[O-])C(C)(C)CC2(C)C
Mol. weight [g/mol]:	278.30
CAS:	116-66-5

Physical Properties

Property code	Value	Unit	Source
gf	254.05	kJ/mol	Joback Method
hf	-80.22	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.770		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1870.60		NIST Webbook
rinpol	1870.60		NIST Webbook
tb	872.55	K	Joback Method
tc	1139.84	K	Joback Method
tf	672.76	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.20	J/mol×K	872.55	Joback Method
cpg	664.76	J/mol×K	917.10	Joback Method
cpg	685.42	J/mol×K	961.65	Joback Method
cpg	707.62	J/mol×K	1006.19	Joback Method
cpg	731.77	J/mol×K	1050.74	Joback Method
cpg	758.29	J/mol×K	1095.29	Joback Method
cpg	787.59	J/mol×K	1139.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116665&Units=SI
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

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

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