Phenol, 2-methyl, 4,6-dinitro-

Other names:

2,4-Dinitro-6-methylphenol
2,4-Dinitro-o-cresol
2-Methyl-4,6-dinitrophenol
3,5-Dinitro-2-hydroxytoluene
4,6-DNOC
4,6-Dinitro-2-methylphenol
4,6-Dinitro-o-cresol
4,6-Dinitro-o-cresolo
4,6-Dinitro-o-kresol
4,6-Dinitrocresol
4,6-Dinitrokresol
6-Methyl-2,4-dinitrophenol
Antinonin
Antinonnin
Arborol
C.I. 10310
Capsine
Chemsect DNOC
DINOK
DNC
Degrassan
Dekrysil
Detal
Detol
Dillex
Dinitro
Dinitro-o-cresol
Dinitrocresol
Dinitrodendtroxal
Dinitrol
Dinitrosol
Dinoc
Dinurania
Ditrosol
Dn
Dn-dry mix no. 2
Dnoc
Dnok
Dwunitro-o-krezol
ENT 154

	Effusan
	Effusan 3436
	Elgetol
	Elgetol 30
	Elgetox
	Elipol
	Extrar
	Flavin-Sandoz
	Hedolit
	Hedolite
	K III
	K IV
	Krenite
	Kresamone
	Kresonite-E
	Krezotol 50
	Le dinitrocresol-4,6
	Lipan
	Nitrador
	Nitrofan
	Oranz viktoria
	Prokarbol
	RCRA Waste number P047
	Rafex
	Rafex 35
	Raphatox
	Sandolin
	Sandolin A
	Selinon
	Sinox
	Trifocide
	Trifrina
	Winterwash
	Zahlreiche bezeichnungen
	o-Cresol, 4,6-dinitro-
Inchi:	InChI=1S/C7H6N2O5/c1-4-2-5(8(11)12)3-6(7(4)10)9(13)14/h2-3,10H,1H3
InchiKey:	ZXVONLUNISGICL-UHFFFAOYSA-N
Formula:	C7H6N2O5
SMILES:	Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	198.13
CAS:	534-52-1

Physical Properties

Property code	Value	Unit	Source
chs	-3332.90	kJ/mol	NIST Webbook
gf	17.69	kJ/mol	Joback Method
hf	-173.05	kJ/mol	Joback Method
hfs	-279.00	kJ/mol	NIST Webbook
hfus	35.65	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-1.46		Estimated Solubility Method
log10ws	-1.46		Aqueous Solubility Prediction Method
logp	1.517		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
rinpol	274.10		NIST Webbook
rinpol	274.10		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1634.60		NIST Webbook
rinpol	1634.60		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	275.47		NIST Webbook
tb	780.50	K	Joback Method
tc	1059.76	K	Joback Method
tf	359.75	K	Aqueous Solubility Prediction Method
tf	360.25 ± 0.20	K	NIST Webbook
tf	359.00 ± 0.20	K	NIST Webbook
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.95	J/mol×K	780.50	Joback Method
cpg	343.28	J/mol×K	827.04	Joback Method

cpg	351.09	J/mol×K	873.59	Joback Method
cpg	358.52	J/mol×K	920.13	Joback Method
cpg	365.69	J/mol×K	966.67	Joback Method
cpg	372.74	J/mol×K	1013.21	Joback Method
cpg	379.80	J/mol×K	1059.76	Joback Method
hfust	19.41	kJ/mol	359.30	NIST Webbook
hfust	19.41	kJ/mol	359.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C534521&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion 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

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