

Phenol, 2-cyclohexyl-4,6-dinitro-

Other names:

Dinex
Dry Mix No. 1
DN Dry Mix No. 1
DN 1
DNOCHP
SN 46
2-Cyclohexyl-4,6-Dinitrophenol
2,4-Dinitro-6-cyclohexylphenol
4,6-Dinitro-o-cyclohexylphenol
Dinitro-o-cyclohexylphenol
Dinitrocyclohexylphenol
Dn dust no. 12
Dowspray 17
ENT 157
Pedinex
Phenol, 6-cyclohexyl-2,4-dinitro-
2-Cyclohexyl-4,6-dinitrofenol
6-Cicloesil-2,4-dinitr-fenolo
6-Cyclohexyl-2,4-dinitrophenol
DN
NA 9026
Rcra waste number P034
DN (pesticide)
NSC 403662

Inchi: InChI=1S/C12H14N2O5/c15-12-10(8-4-2-1-3-5-8)6-9(13(16)17)7-11(12)14(18)19/h6-8,15

InchiKey: QJYHUJAGJUHXJN-UHFFFAOYSA-N

Formula: C12H14N2O5

SMILES: O=[N+](O)c1cc(C2CCCCC2)c(O)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 266.25

CAS: 131-89-5

Physical Properties

Property code	Value	Unit	Source
gf	84.24	kJ/mol	Joback Method
hf	-221.93	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method

hvap	92.53	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.256		Crippen Method
mcvol	186.030	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	914.45	K	Joback Method
tc	1200.95	K	Joback Method
tf	378.70 ± 0.20	K	NIST Webbook
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.13	J/mol×K	914.45	Joback Method
cpg	604.10	J/mol×K	962.20	Joback Method
cpg	616.24	J/mol×K	1009.95	Joback Method
cpg	627.72	J/mol×K	1057.70	Joback Method
cpg	638.74	J/mol×K	1105.45	Joback Method
cpg	649.49	J/mol×K	1153.20	Joback Method
cpg	660.15	J/mol×K	1200.95	Joback Method
hfust	28.03	kJ/mol	378.70	NIST Webbook
hvapt	88.60	kJ/mol	485.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C131895&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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