4-Nitrocatechol

Other names:	4-Nitropyrocatechol
	1,2-Benzenediol, 4-nitro-
Inchi:	InChI=1S/C6H5NO4/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3,8-9H
InchiKey:	XJNPNXSISMKQEX-UHFFFAOYSA-N
Formula:	C6H5NO4
SMILES:	O=[N+]([O-])c1ccc(O)c(O)c1
Mol. weight [g/mol]:	155.11
CAS:	3316-09-4

Physical Properties

Property code	Value	Unit	Source
chs	-2664.50 ± 0.80	kJ/mol	NIST Webbook
gf	-161.64	kJ/mol	Joback Method
hf	-290.00 ± 1.80	kJ/mol	NIST Webbook
hfs	-411.10 ± 1.10	kJ/mol	NIST Webbook
hfus	28.26	kJ/mol	Joback Method
hsub	121.10 ± 1.40	kJ/mol	NIST Webbook
hvap	73.84	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.006		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	7522.14	kPa	Joback Method
tb	676.44	K	Joback Method
tc	949.68	K	Joback Method
tf	550.85	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.15	J/mol×K	676.44	Joback Method
cpg	261.22	J/mol×K	721.98	Joback Method
cpg	267.80	J/mol×K	767.52	Joback Method
cpg	274.10	J/mol×K	813.06	Joback Method

cpg	280.31	J/mol×K	858.60	Joback Method
cpg	286.67	J/mol×K	904.14	Joback Method
cpg	293.36	J/mol×K	949.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3316094&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

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

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