

Nitrobenzene-D5

Other names:	Benzene-D5-, nitro-[2H5]Benzene, nitro-nitro(2H5)benzene
Inchi:	InChI=1S/C6H5NO2/c8-7(9)6-4-2-1-3-5-6/h1-5H/i1D,2D,3D,4D,5D
InchiKey:	LQNUZADURLCDLV-RALIUCGRSA-N
Formula:	C6D5NO2
SMILES:	O=[N+](O-)c1ccccc1
Mol. weight [g/mol]:	128.14
CAS:	4165-60-0

Physical Properties

Property code	Value	Unit	Source
ea	1.00 ± 0.02	eV	NIST Webbook
ea	1.00 ± 0.10	eV	NIST Webbook
gf	147.60	kJ/mol	Joback Method
hf	58.60	kJ/mol	Joback Method
hfus	16.70	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.595		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
rinpol	179.50		NIST Webbook
rinpol	179.50		NIST Webbook
tb	515.20	K	Joback Method
tc	769.26	K	Joback Method
tf	327.41	K	Joback Method
vc	0.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.20	J/mol×K	515.20	Joback Method
cpg	190.50	J/mol×K	557.54	Joback Method

cpg	199.95	J/mol×K	599.89	Joback Method
cpg	208.60	J/mol×K	642.23	Joback Method
cpg	216.51	J/mol×K	684.57	Joback Method
cpg	223.71	J/mol×K	726.92	Joback Method
cpg	230.26	J/mol×K	769.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4165600&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
ea:	Electron affinity
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

Latest version available from:

<https://www.chemeo.com/cid/19-391-7/Nitrobenzene-D5.pdf>

Generated by Cheméo on 2024-04-19 18:03:02.985219796 +0000 UTC m=+15839031.905797120.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.