

Phenol, 2-(1,1-dimethylethyl)-4-nitro

Inchi:	InChI=1S/C10H13NO3/c1-10(2,3)8-6-7(11(13)14)4-5-9(8)12/h4-6,12H,1-3H3
InchiKey:	WPLSSAJHDAQNCO-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	CC(C)(C)c1cc([N+](=O)[O-])ccc1O
Mol. weight [g/mol]:	195.22

Physical Properties

Property code	Value	Unit	Source
gf	19.87	kJ/mol	Joback Method
hf	-221.49	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.598		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1782.00		NIST Webbook
tb	689.09	K	Joback Method
tc	946.78	K	Joback Method
tf	499.15	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.40	J/mol×K	689.09	Joback Method
cpg	420.93	J/mol×K	732.04	Joback Method
cpg	432.51	J/mol×K	774.99	Joback Method
cpg	443.29	J/mol×K	817.94	Joback Method
cpg	453.43	J/mol×K	860.88	Joback Method
cpg	463.09	J/mol×K	903.83	Joback Method
cpg	472.43	J/mol×K	946.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R58589&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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