

2-NITROCUMENE

Other names:	1-Isopropyl-2-nitrobenzene 1-Nitro-2-isopropylbenzene 2-Isopropylnitrobenzene 2-Nitroisopropylbenzene Benzene, 1-(1-methylethyl)-2-nitro- Cumene, o-nitro- o-Isopropylnitrobenzene o-Nitrocumene o-Nitroisopropylbenzene
Inchi:	InChI=1S/C9H11NO2/c1-7(2)8-5-3-4-6-9(8)10(11)12/h3-7H,1-2H3
InchiKey:	BSMKYQUHXQAVKG-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CC(C)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	165.19
CAS:	6526-72-3

Physical Properties

Property code	Value	Unit	Source
hf	-14.44	kJ/mol	Cheméo Relay (1.0)
hfus	20.56	kJ/mol	Joback Method
hvap	65.60 ± 0.70	kJ/mol	NIST Webbook
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-3.60		Cheméo Relay (1.0)
logp	2.718		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	521.80	K	Cheméo Relay (1.0)
tc	755.79	K	Cheméo Relay (1.0)
tf	286.66	K	Cheméo Relay (1.0)
vc	0.454	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	311.23	J/mol×K	588.38	Joback Method
cpg	324.77	J/mol×K	629.21	Joback Method
cpg	337.33	J/mol×K	670.03	Joback Method
cpg	348.96	J/mol×K	710.86	Joback Method
cpg	359.71	J/mol×K	751.69	Joback Method
cpg	369.63	J/mol×K	792.51	Joback Method
cpg	378.76	J/mol×K	833.34	Joback Method
hvapt	65.50 ± 0.70	kJ/mol	300.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43515e+01
Coeff. B	-4.36379e+03
Coeff. C	-8.78370e+01
Temperature range (K), min.	398.12
Temperature range (K), max.	570.56

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6526723&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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