

1-NITRO-2-PROPYLBENZENE

Other names:	Benzene, 1-nitro-2-propyl- o-Propylnitrobenzene o-Nitropropylbenzene
Inchi:	InChI=1S/C9H11NO2/c1-2-5-8-6-3-4-7-9(8)10(11)12/h3-4,6-7H,2,5H2,1H3
InchiKey:	UGAXDAGIKIVCQB-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	165.19

Physical Properties

Property code	Value	Unit	Source
af	0.5374		Cheméo Relay (1.0)
hf	-2.21	kJ/mol	Cheméo Relay (1.0)
hfus	24.08	kJ/mol	Joback Method
hvap	62.06	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.547		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
ripol	1969.00		NIST Webbook
tb	530.80	K	Cheméo Relay (1.0)
tc	758.21	K	Cheméo Relay (1.0)
tf	269.05	K	Cheméo Relay (1.0)
vc	0.461	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.78	J/mol×K	588.82	Joback Method
cpg	323.96	J/mol×K	628.74	Joback Method
cpg	336.22	J/mol×K	668.66	Joback Method
cpg	347.61	J/mol×K	708.57	Joback Method
cpg	358.16	J/mol×K	748.49	Joback Method

cpg	367.92	J/mol×K	788.41	Joback Method
cpg	376.94	J/mol×K	828.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.70	K	3.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7137544&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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