1-NITRO-4-PROPYLBENZENE

Other names: 4-Nitro-n-propylbenzene
Benzene, 1-nitro-4-propyl-
p-Propylnitrobenzene
p-Nitropropylbenzene
Inchi: InChI=1S/C9H11NO2/c1-2-3-8-4-6-9(7-5-8)10(11)12/h4-7H,2-3H2,1H3
InchiKey: SXQBFCVVZIYXHV-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CCCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
af	0.5543		Cheméo Relay (1.0)
gf	163.23	kJ/mol	Joback Method
hf	-4.52	kJ/mol	Cheméo Relay (1.0)
hfus	24.08	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-3.71		Cheméo Relay (1.0)
logp	2.547		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
ripol	2135.00		NIST Webbook
ripol	2135.00		NIST Webbook
tb	533.11	K	Cheméo Relay (1.0)
tc	760.69	K	Cheméo Relay (1.0)
tf	296.64	K	Cheméo Relay (1.0)
vc	0.465	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

Sources

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
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=C10342593&Units=SI

Legend

af:	Acentric Factor
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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