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
CAS:	10342-59-3

Physical Properties

Property code	Value	Unit	Source
gf	163.23	kJ/mol	Joback Method
hf	-14.79	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
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	588.82	K	Joback Method
tc	828.33	K	Joback Method
tf	373.74	K	Joback Method
vc	0.513	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10342593&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume