o-nitrobutylbenzene

Other names:	Benzene, 1-butyl-2-nitro-
	1-butyl-2-nitrobenzene
Inchi:	InChI=1S/C10H13NO2/c1-2-3-6-9-7-4-5-8-10(9)11(12)13/h4-5,7-8H,2-3,6H2,1H3
InchiKey:	RSVIEXUVWMYRGB-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	179.22
CAS:	7137-55-5

Physical Properties

Property code	Value	Unit	Source
gf	171.65	kJ/mol	Joback Method
hf	-35.43	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.937		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
ripol	2056.00		NIST Webbook
tb	611.70	K	Joback Method
tc	846.29	K	Joback Method
tf	385.01	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.03	J/mol×K	611.70	Joback Method
cpg	372.01	J/mol×K	650.80	Joback Method
cpg	385.03	J/mol×K	689.90	Joback Method
cpg	397.15	J/mol×K	728.99	Joback Method
cpg	408.40	J/mol×K	768.09	Joback Method
cpg	418.84	J/mol×K	807.19	Joback Method

cpg	428.50	J/mol×K	846.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7137555&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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