

p-Butoxybenzonitrile

Other names:	4-(n-Butoxy)benzonitrile Benzonitrile, 4-butoxy-
Inchi:	InChI=1S/C11H13NO/c1-2-3-8-13-11-6-4-10(9-12)5-7-11/h4-7H,2-3,8H2,1H3
InchiKey:	RRGQINKVTNAIBB-UHFFFAOYSA-N
Formula:	C11H13NO
SMILES:	CCCCOc1ccc(C#N)cc1
Mol. weight [g/mol]:	175.23
CAS:	5203-14-5

Physical Properties

Property code	Value	Unit	Source
gf	172.70	kJ/mol	Joback Method
hf	-12.65	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.737		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	607.24	K	Joback Method
tc	824.82	K	Joback Method
tf	339.89	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.61	J/mol×K	607.24	Joback Method
cpg	370.49	J/mol×K	643.50	Joback Method
cpg	382.63	J/mol×K	679.77	Joback Method
cpg	394.05	J/mol×K	716.03	Joback Method
cpg	404.75	J/mol×K	752.29	Joback Method
cpg	414.76	J/mol×K	788.56	Joback Method
cpg	424.10	J/mol×K	824.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.50 ± 0.50	K	0.01	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5203145&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/49-584-0/p-Butoxybenzonitrile.pdf>

Generated by Cheméo on 2025-12-21 21:28:16.289193274 +0000 UTC m=+6100693.819233928.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.