

p-Pentyloxynitrobenzene

Other names:	Benzene, 1-nitro-4-pentyloxy p-Nitrophenyl pentyl ether
Inchi:	InChI=1S/C11H15NO3/c1-2-3-4-9-15-11-7-5-10(6-8-11)12(13)14/h5-8H,2-4,9H2,1H3
InchiKey:	ITRUYFFRYGZFBF-UHFFFAOYSA-N
Formula:	C11H15NO3
SMILES:	CCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	209.24
CAS:	63469-11-4

Physical Properties

Property code	Value	Unit	Source
gf	75.07	kJ/mol	Joback Method
hf	-188.29	kJ/mol	Joback Method
hfus	30.45	kJ/mol	Joback Method
hvap	62.02	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.164		Crippen Method
mvol	165.380	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	657.00	K	Joback Method
tc	883.75	K	Joback Method
tf	418.51	K	Joback Method
vc	0.643	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.88	J/molxK	657.00	Joback Method
cpg	446.22	J/molxK	694.79	Joback Method
cpg	459.61	J/molxK	732.58	Joback Method
cpg	472.10	J/molxK	770.38	Joback Method
cpg	483.70	J/molxK	808.17	Joback Method
cpg	494.45	J/molxK	845.96	Joback Method
cpg	504.37	J/molxK	883.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	466.50 ± 1.50	K	2.10	NIST Webbook

Sources

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=C63469114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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