

p-Hexyloxy nitrobenzene

Other names:	Benzene, 1-(hexyloxy)-4-nitro- 1-(Hexyloxy)-4-nitrobenzene p-Nitrophenyl hexyl ether
Inchi:	InChI=1S/C12H17NO3/c1-2-3-4-5-10-16-12-8-6-11(7-9-12)13(14)15/h6-9H,2-5,10H2,1H3
InchiKey:	VLMYJULPWGTTAV-UHFFFAOYSA-N
Formula:	C12H17NO3
SMILES:	CCCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	223.27
CAS:	15440-98-9

Physical Properties

Property code	Value	Unit	Source
gf	83.49	kJ/mol	Joback Method
hf	-208.93	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.554		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	679.88	K	Joback Method
tc	902.53	K	Joback Method
tf	429.78	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.95	J/molxK	679.88	Joback Method
cpg	497.82	J/molxK	716.99	Joback Method
cpg	511.73	J/molxK	754.10	Joback Method
cpg	524.70	J/molxK	791.21	Joback Method
cpg	536.76	J/molxK	828.32	Joback Method
cpg	547.94	J/molxK	865.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	476.50 ± 0.50	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15440989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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