P-HEXYLOXYNITROBENZENE

Other names: 1-(Hexyloxy)-4-nitrobenzene
Benzene, 1-(hexyloxy)-4-nitro-
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

Physical Properties

Property code	Value	Unit	Source
hf	-208.64	kJ/mol	Cheméo Relay (1.0)
hfus	33.04	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-4.83		Cheméo Relay (1.0)
logp	3.554		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
tb	583.76	K	Cheméo Relay (1.0)
tf	314.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.95	J/mol×K	679.88	Joback Method
cpg	497.82	J/mol×K	716.99	Joback Method
cpg	511.73	J/mol×K	754.10	Joback Method
cpg	524.70	J/mol×K	791.21	Joback Method
cpg	536.76	J/mol×K	828.32	Joback Method
cpg	547.94	J/mol×K	865.42	Joback Method
cpg	558.27	J/mol×K	902.53	Joback Method

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15440989&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point