p-Nitrophenyloctyl ether

Other names: p-Nitrophenyl octyl ether
Inchi: InChI=1S/C14H21NO3/c1-2-3-4-5-6-7-12-18-14-10-8-13(9-11-14)15(16)17/h8-11H,2-7,1
InchiKey: WTTNDGCMXADGCJ-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CCCCCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 251.33

Physical Properties

Property code	Value	Unit	Source
hf	-252.74	kJ/mol	Cheméo Relay (1.0)
hfus	38.22	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-5.56		Cheméo Relay (1.0)
logp	4.334		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
tb	600.75	K	Cheméo Relay (1.0)
tf	316.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.01	J/mol×K	725.64	Joback Method
cpg	604.71	J/mol×K	761.58	Joback Method
cpg	619.39	J/mol×K	797.51	Joback Method
cpg	633.10	J/mol×K	833.45	Joback Method
cpg	645.85	J/mol×K	869.39	Joback Method
cpg	657.69	J/mol×K	905.32	Joback Method
cpg	668.66	J/mol×K	941.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	496.00 ± 1.00	K	2.00	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49562767&Units=SI

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