5-Benzyloxy-2-nitrotoluene

Other names: Benzene, 2-methyl-1-nitro-4-(phenylmethoxy)-
Ether, benzyl 4-nitro-m-tolyl-
Inchi: InChI=1S/C14H13NO3/c1-11-9-13(7-8-14(11)15(16)17)18-10-12-5-3-2-4-6-12/h2-9H,10H
InchiKey: PBAXHOUGHZKSRP-UHFFFAOYSA-N
Formula: C14H13NO3
SMILES: Cc1cc(OCc2ccccc2)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 243.26
CAS: 22424-58-4

Physical Properties

Property code	Value	Unit	Source
gf	203.11	kJ/mol	Joback Method
hf	-25.15	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	71.64	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.482		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	757.30	K	Joback Method
tc	1015.22	K	Joback Method
tf	491.26	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.29	J/mol×K	757.30	Joback Method
cpg	513.38	J/mol×K	800.29	Joback Method
cpg	526.21	J/mol×K	843.27	Joback Method
cpg	537.83	J/mol×K	886.26	Joback Method
cpg	548.30	J/mol×K	929.25	Joback Method
cpg	557.69	J/mol×K	972.24	Joback Method
cpg	566.05	J/mol×K	1015.22	Joback Method

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=C22424584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume