4'-Nitrobenzo-15-crown-5

Other names: 17-Nitro-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadecen-2
Inchi: InChI=1S/C14H19NO7/c16-15(17)12-1-2-13-14(11-12)22-10-8-20-6-4-18-3-5-19-7-9-21-
InchiKey: XIWRBQVYCZCEPG-UHFFFAOYSA-N
Formula: C14H19NO7
SMILES: O=[N+]([O-])c1ccc2c(c1)OCCOCCOCCOCCO2
Mol. weight [g/mol]: 313.30
CAS: 60835-69-0

Physical Properties

Property code	Value	Unit	Source
gf	-287.44	kJ/mol	Joback Method
hf	-757.92	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.416		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	897.06	K	Joback Method
tc	1183.31	K	Joback Method
tf	562.44	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.47	J/mol×K	897.06	Joback Method
cpg	738.77	J/mol×K	944.77	Joback Method
cpg	750.17	J/mol×K	992.48	Joback Method
cpg	758.63	J/mol×K	1040.18	Joback Method
cpg	764.10	J/mol×K	1087.89	Joback Method
cpg	766.55	J/mol×K	1135.60	Joback Method
cpg	765.93	J/mol×K	1183.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60835690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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