

17-NITRO-2,3-BENZO-1,4,7,10,13-PENTAOXACYC

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]:	313.31

Physical Properties

Property code	Value	Unit	Source
hf	-673.21	kJ/mol	Cheméo Relay (1.0)
hfus	52.60	kJ/mol	Joback Method
hvap	112.42	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	1.416		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
tb	698.61	K	Cheméo Relay (1.0)
tf	371.78	K	Cheméo Relay (1.0)

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

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=C60835690&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tf:	Normal melting (fusion) point

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