KRYPTOFIX-221

Other names: 4,7,13,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5.]tricosane
Kryptofix 221
4,7,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5.]tricosane
Inchi: InChI=1S/C16H32N2O5/c1-7-19-8-2-18-5-11-22-15-13-20-9-3-17(1)4-10-21-14-16-23-12
InchiKey: HDLXPNDSLDLJHF-UHFFFAOYSA-N
Formula: C16H32N2O5
SMILES: C1COCCN2CCOCCOCCN(CCO1)CCOCC2
Mol. weight [g/mol]: 332.44

Physical Properties

Property code	Value	Unit	Source
af	0.5615		Cheméo Relay (1.0)
gf	-42.05	kJ/mol	Cheméo Relay (1.0, beta)
hf	-831.92	kJ/mol	Cheméo Relay (1.0)
hvap	105.76	kJ/mol	Cheméo Relay (1.0)
ie	7.40	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	0.65		Cheméo Relay (1.0)
logp	-0.299		Crippen Method
mcvol	263.890	ml/mol	McGowan Method
pc	1307.12	kPa	Cheméo Relay (1.0, beta)
tb	703.13	K	Cheméo Relay (1.0)
tc	927.29	K	Cheméo Relay (1.0)
tf	392.19	K	Cheméo Relay (1.0)
vc	0.874	m3/kmol	Cheméo Relay (1.0)

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=C31364428&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume