4,7,13-Trioxa-1,10-diazacyclopentadecane

Other names:	1,4,10-Trioxa-7,13-diazacyclopentadecane
	Kryptofix 21
	1,7,10-Trioxa-4,13-diazacyclopentadecane
Inchi:	InChI=1S/C10H22N2O3/c1-5-13-6-2-12-4-8-15-10-9-14-7-3-11-1/h11-12H,1-10H2
InchiKey:	STHIZMRUXPMSCW-UHFFFAOYSA-N
Formula:	C10H22N2O3
SMILES:	C1COCCNCCOCCOCCN1
Mol. weight [g/mol]:	218.29
CAS:	31249-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-126.36	kJ/mol	Joback Method
hf	-550.89	kJ/mol	Joback Method
hfus	36.64	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	0.46		Crippen Method
logp	-0.771		Crippen Method
mcvol	178.470	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	668.80	K	Joback Method
tc	942.22	K	Joback Method
tf	472.17	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.05	J/mol×K	668.80	Joback Method
cpg	544.83	J/mol×K	714.37	Joback Method
cpg	568.38	J/mol×K	759.94	Joback Method
cpg	589.57	J/mol×K	805.51	Joback Method

cpg	608.29	J/mol×K	851.08	Joback Method
cpg	624.40	J/mol×K	896.65	Joback Method
cpg	637.80	J/mol×K	942.22	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=C31249953&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
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