

1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane

Other names:

4,7,13,16-Tetraoxa-1,10-diazacyclooctadecane
1,10-Diaza-18-crown-6
Kryptofix 22
Diaza-18-crown-6
Kryptofix[2.2]
1,7,10,16-Tetraoxa-4,13-diazacyclooctadecane
1,10-Diaza-4,7,13,16-tetraoxacyclooctadecane
7,16-Diaza-18-crown-6
Cryptand 22
NSC 339325

Inchi:

InChI=1S/C12H26N2O4/c1-5-15-9-10-17-7-3-14-4-8-18-12-11-16-6-2-13-1/h13-14H,1-12

InchiKey:

NLMDJJTUQPXZFG-UHFFFAOYSA-N

Formula:

C₁₂H₂₆N₂O₄

SMILES:

C1COCCOCCNCCOCCOCCN1

Mol. weight [g/mol]:

262.35

CAS:

23978-55-4

Physical Properties

Property code	Value	Unit	Source
gf	-231.94	kJ/mol	Joback Method
hf	-742.65	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	0.53		Crippen Method
logp	-0.754		Crippen Method
mvol	212.520	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	754.32	K	Joback Method
tc	1035.56	K	Joback Method
tf	510.72	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.26	J/molxK	754.32	Joback Method
cpg	704.63	J/molxK	801.19	Joback Method
cpg	727.79	J/molxK	848.07	Joback Method
cpg	747.58	J/molxK	894.94	Joback Method
cpg	763.80	J/molxK	941.81	Joback Method
cpg	776.28	J/molxK	988.68	Joback Method
cpg	784.84	J/molxK	1035.56	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=C23978554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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