

1,3,6,9,12,14,17,20-Octaoxacyclodocosane

Inchi:	InChI=1S/C14H28O8/c1-2-16-6-10-20-14-22-12-8-18-4-3-17-7-11-21-13-19-9-5-15-1/h1-
InchiKey:	DGVSCNPOZONLEG-UHFFFAOYSA-N
Formula:	C14H28O8
SMILES:	C1COCCOCOCOCOCOCOCOCOCOC1
Mol. weight [g/mol]:	324.37
CAS:	74485-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-783.40	kJ/mol	Joback Method
hf	-1412.19	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	86.33	kJ/mol	Joback Method
log10ws	0.73		Crippen Method
logp	0.048		Crippen Method
mcvol	244.220	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	827.86	K	Joback Method
tc	1108.16	K	Joback Method
tf	415.40	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.02	J/mol×K	827.86	Joback Method
cpg	863.30	J/mol×K	874.58	Joback Method
cpg	882.42	J/mol×K	921.29	Joback Method
cpg	897.18	J/mol×K	968.01	Joback Method
cpg	907.35	J/mol×K	1014.73	Joback Method
cpg	912.71	J/mol×K	1061.44	Joback Method
cpg	913.05	J/mol×K	1108.16	Joback Method
dvisc	0.0011001	Pa×s	415.40	Joback Method
dvisc	0.0000929	Pa×s	484.14	Joback Method

dvisc	0.0000145	Pa×s	552.89	Joback Method
dvisc	0.0000034	Pa×s	621.63	Joback Method
dvisc	0.0000011	Pa×s	690.37	Joback Method
dvisc	0.0000004	Pa×s	759.12	Joback Method
dvisc	0.0000002	Pa×s	827.86	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=C74485420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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