

I,3,6-Trioxocane

Other names:	Diethylene glycol formal Diglycol formal 1,3,6-Trioxacyclooctane 1,3,6-Trioxocin, tetrahydro- I,3,6-Trioxocane
Inchi:	InChI=1S/C5H10O3/c1-3-7-5-8-4-2-6-1/h1-5H2
InchiKey:	AUAGGMPIKOZAJZ-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	C1COCOCCO1
Mol. weight [g/mol]:	118.13

Physical Properties

Property code	Value	Unit	Source
af	0.3076		Cheméo Relay (1.0)
chl	-2880.75 ± 0.99	kJ/mol	NIST Webbook
gf	-259.18	kJ/mol	Joback Method
hf	-467.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-516.00 ± 1.20	kJ/mol	NIST Webbook
hfus	19.21	kJ/mol	Joback Method
hvap	48.80	kJ/mol	NIST Webbook
hvap	48.80 ± 0.20	kJ/mol	NIST Webbook
hvap	48.77	kJ/mol	NIST Webbook
hvap	48.77 ± 0.21	kJ/mol	NIST Webbook
ie	9.23	eV	NIST Webbook
log10ws	0.81		Cheméo Relay (1.0)
logp	0.007		Crippen Method
mcvol	88.060	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	433.51	K	Cheméo Relay (1.0)
tc	629.66	K	Cheméo Relay (1.0)
tf	249.80	K	Cheméo Relay (1.0)
vc	0.310	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.95	J/mol×K	427.41	Joback Method
cpg	193.11	J/mol×K	465.04	Joback Method
cpg	206.55	J/mol×K	502.68	Joback Method
cpg	219.29	J/mol×K	540.31	Joback Method
cpg	231.33	J/mol×K	577.95	Joback Method
cpg	242.65	J/mol×K	615.58	Joback Method
cpg	253.27	J/mol×K	653.22	Joback Method
dvisc	0.0311861	Pa×s	230.40	Joback Method
dvisc	0.0091718	Pa×s	263.24	Joback Method
dvisc	0.0035387	Pa×s	296.07	Joback Method
dvisc	0.0016512	Pa×s	328.90	Joback Method
dvisc	0.0008848	Pa×s	361.74	Joback Method
dvisc	0.0005260	Pa×s	394.57	Joback Method
dvisc	0.0003388	Pa×s	427.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C1779197&Units=SI

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfl:	Liquid phase 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

Latest version available from:

<https://www.cheméo.com/cid/45-898-6/l-3-6-Trioxocane.pdf>

Generated by Cheméo on 2026-07-21 19:59:05.070774683 +0000 UTC m=+175040.912660061.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.