

3,6,9,12-Tetraoxatetradecane-1,14-diol, diacetate

Other names:	3,6,9,12-tetraoxatetradecane-1,14-diyl diacetate
Inchi:	InChI=1S/C14H26O8/c1-13(15)21-11-9-19-7-5-17-3-4-18-6-8-20-10-12-22-14(2)16/h3-12
InchiKey:	MBGINZGOPMLHQN-UHFFFAOYSA-N
Formula:	C14H26O8
SMILES:	CC(=O)OCCOCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]:	322.35
CAS:	22790-13-2

Physical Properties

Property code	Value	Unit	Source
gf	-820.84	kJ/mol	Joback Method
hf	-1350.77	kJ/mol	Joback Method
hfus	42.34	kJ/mol	Joback Method
hvap	74.71	kJ/mol	Joback Method
log10ws	0.24		Crippen Method
logp	0.179		Crippen Method
mcvol	246.480	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	761.98	K	Joback Method
tc	941.91	K	Joback Method

tf	480.78	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.94	J/mol×K	761.98	Joback Method
cpg	803.55	J/mol×K	911.92	Joback Method
cpg	792.31	J/mol×K	881.93	Joback Method
cpg	780.10	J/mol×K	851.94	Joback Method
cpg	766.95	J/mol×K	821.96	Joback Method
cpg	752.88	J/mol×K	791.97	Joback Method
cpg	813.79	J/mol×K	941.91	Joback Method
dvisc	0.0000401	Paxs	761.98	Joback Method
dvisc	0.0000512	Paxs	715.11	Joback Method
dvisc	0.0000677	Paxs	668.25	Joback Method
dvisc	0.0000935	Paxs	621.38	Joback Method
dvisc	0.0001359	Paxs	574.51	Joback Method
dvisc	0.0002113	Paxs	527.65	Joback Method
dvisc	0.0003580	Paxs	480.78	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=C22790132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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