

Benzene, (triethoxymethyl)-

Other names:	Orthobenzoic acid, triethyl ester Ethyl orthobenzoate Triethyl orthobenzoate (triethoxymethyl)benzene
Inchi:	InChI=1S/C13H20O3/c1-4-14-13(15-5-2,16-6-3)12-10-8-7-9-11-12/h7-11H,4-6H2,1-3H3
InchiKey:	BQFPCTXLBRVFJL-UHFFFAOYSA-N
Formula:	C13H20O3
SMILES:	CCOC(OCC)(OCC)c1ccccc1
Mol. weight [g/mol]:	224.30
CAS:	1663-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-141.17	kJ/mol	Joback Method
hf	-480.53	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.906		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
tb	513.20	K	NIST Webbook
tc	790.45	K	Joback Method
tf	331.80	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.72	J/molxK	587.55	Joback Method
cpg	554.90	J/molxK	756.63	Joback Method
cpg	541.27	J/molxK	722.82	Joback Method
cpg	526.76	J/molxK	689.00	Joback Method
cpg	511.34	J/molxK	655.18	Joback Method

cpg	495.00	J/mol×K	621.37	Joback Method
cpg	567.66	J/mol×K	790.45	Joback Method
dvisc	0.0000923	Paxs	587.55	Joback Method
dvisc	0.0001233	Paxs	544.92	Joback Method
dvisc	0.0001730	Paxs	502.30	Joback Method
dvisc	0.0002584	Paxs	459.67	Joback Method
dvisc	0.0004191	Paxs	417.05	Joback Method
dvisc	0.0007588	Paxs	374.43	Joback Method
dvisc	0.0016002	Paxs	331.80	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=C1663612&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
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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