

Ethane, 1,1,1-trichloro-2,2-diethoxy-

Inchi:	InChI=1S/C6H11Cl3O2/c1-3-10-5(11-4-2)6(7,8)9/h5H,3-4H2,1-2H3
InchiKey:	CGCJBAIEQANINV-UHFFFAOYSA-N
Formula:	C6H11Cl3O2
SMILES:	CCOC(OCC)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	221.51
CAS:	599-97-3

Physical Properties

Property code	Value	Unit	Source
gf	-245.75	kJ/mol	Joback Method
hf	-492.86	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.756		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	490.14	K	Joback Method
tc	691.29	K	Joback Method
tf	279.02	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.47	J/molxK	490.14	Joback Method
cpg	295.07	J/molxK	523.66	Joback Method
cpg	305.13	J/molxK	557.19	Joback Method
cpg	314.66	J/molxK	590.71	Joback Method
cpg	323.68	J/molxK	624.24	Joback Method
cpg	332.19	J/molxK	657.76	Joback Method
cpg	340.20	J/molxK	691.29	Joback Method
dvisc	0.0040650	Paxs	279.02	Joback Method
dvisc	0.0018872	Paxs	314.21	Joback Method

dvisc	0.0010225	Paxs	349.39	Joback Method
dvisc	0.0006198	Paxs	384.58	Joback Method
dvisc	0.0004086	Paxs	419.77	Joback Method
dvisc	0.0002873	Paxs	454.95	Joback Method
dvisc	0.0002124	Paxs	490.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	1.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C599973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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