

Ethanol-d1

Other names:	ethanol-1-d
Inchi:	InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3/i1D
InchiKey:	LFQSCWFLJHTTHZ-MICDWDOJSA-N
Formula:	C2H5DO
SMILES:	CCO
Mol. weight [g/mol]:	47.07
CAS:	1624-36-8

Physical Properties

Property code	Value	Unit	Source
gf	-170.86	kJ/mol	Joback Method
hf	-236.84	kJ/mol	Joback Method
hfus	5.02	kJ/mol	Joback Method
hvap	36.73	kJ/mol	Joback Method
log10ws	0.08		Crippen Method
logp	-0.001		Crippen Method
mcvol	44.910	ml/mol	McGowan Method
pc	5756.64	kPa	Joback Method
tb	337.34	K	Joback Method
tc	499.11	K	Joback Method
tf	173.12	K	Joback Method
vc	0.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	83.09	J/molxK	418.23	Joback Method
cpg	75.12	J/molxK	364.30	Joback Method
cpg	70.94	J/molxK	337.34	Joback Method
cpg	86.89	J/molxK	445.19	Joback Method
cpg	90.56	J/molxK	472.15	Joback Method
cpg	94.11	J/molxK	499.11	Joback Method
cpg	79.17	J/molxK	391.26	Joback Method
cpl	102.09	J/molxK	250.00	NIST Webbook

cpl	116.23	J/molxK	298.00	NIST Webbook
dvisc	0.0004219	Paxs	337.34	Joback Method
dvisc	0.0015078	Paxs	282.60	Joback Method
dvisc	0.0034990	Paxs	255.23	Joback Method
dvisc	0.0099391	Paxs	227.86	Joback Method
dvisc	0.0375449	Paxs	200.49	Joback Method
dvisc	0.0007539	Paxs	309.97	Joback Method
dvisc	0.2159052	Paxs	173.12	Joback Method
rhoI	783.63	kg/m3	318.15	Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K
rhoI	801.57	kg/m3	298.15	Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K
rhoI	810.32	kg/m3	288.15	Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K
rhoI	818.95	kg/m3	278.15	Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K
rhoI	792.68	kg/m3	308.15	Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric properties of dilute solutions of water in ethanol and water-d2 in ethanol-d1 between T = (278.15 and 318.15) K:	https://www.doi.org/10.1016/j.jct.2011.10.009
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=C1624368&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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