Ethanol-1,1-d2

Inchi: InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3/i2D2
InchiKey: LFQSCWFLJHTTHZ-CBTSVUPCSA-N
Formula: C2H4D2O
SMILES: CCO
Mol. weight [g/mol]: 48.08
CAS: 1859-09-2

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	70.94	J/mol×K	337.34	Joback Method
cpg	75.12	J/mol×K	364.30	Joback Method
cpg	79.17	J/mol×K	391.26	Joback Method
cpg	83.09	J/mol×K	418.23	Joback Method
cpg	86.89	J/mol×K	445.19	Joback Method
cpg	90.56	J/mol×K	472.15	Joback Method
cpg	94.11	J/mol×K	499.11	Joback Method
dvisc	0.2159052	Pa×s	173.12	Joback Method
dvisc	0.0375449	Pa×s	200.49	Joback Method

dvisc	0.0099391	Pa×s	227.86	Joback Method
dvisc	0.0034990	Pa×s	255.23	Joback Method
dvisc	0.0015078	Pa×s	282.60	Joback Method
dvisc	0.0007539	Pa×s	309.97	Joback Method
dvisc	0.0004219	Pa×s	337.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1859092&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume