

C2H3D3O

Inchi:	InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3/i1D3
InchiKey:	LFQSCWFLJHTTHZ-FIBGUPNXSA-N
Formula:	C2H3D3O
SMILES:	CCO
Mol. weight [g/mol]:	49.09
CAS:	1759-87-1

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/molxK	337.34	Joback Method
cpg	90.56	J/molxK	472.15	Joback Method
cpg	86.89	J/molxK	445.19	Joback Method
cpg	83.09	J/molxK	418.23	Joback Method
cpg	79.17	J/molxK	391.26	Joback Method
cpg	75.12	J/molxK	364.30	Joback Method
cpg	94.11	J/molxK	499.11	Joback Method
dvisc	0.0004219	Paxs	337.34	Joback Method
dvisc	0.0007539	Paxs	309.97	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	0.2159052	Paxs	173.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1759871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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