Ethanol, 2-iodo-

Other names: Ethylene iodohydrin
Iodoethanol
2-Iodoethanol
Inchi: InChI=1S/C2H5IO/c3-1-2-4/h4H,1-2H2
InchiKey: QSECPQCFCWVBKM-UHFFFAOYSA-N
Formula: C2H5IO
SMILES: OCCI
Mol. weight [g/mol]: 171.97
CAS: 624-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-112.74	kJ/mol	Joback Method
hf	-159.97	kJ/mol	Joback Method
hfus	9.43	kJ/mol	Joback Method
hvap	46.10	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.66 ± 0.07	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.414		Crippen Method
mcvol	70.730	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	430.48	K	Joback Method
tc	628.94	K	Joback Method
tf	231.18	K	Joback Method
vc	0.255	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.40	J/mol×K	430.48	Joback Method

cpg	105.65	J/mol×K	463.56	Joback Method
cpg	109.65	J/mol×K	496.63	Joback Method
cpg	113.42	J/mol×K	529.71	Joback Method
cpg	116.98	J/mol×K	562.79	Joback Method
cpg	120.33	J/mol×K	595.86	Joback Method
cpg	123.51	J/mol×K	628.94	Joback Method
dvisc	0.0742348	Pa×s	231.18	Joback Method
dvisc	0.0183302	Pa×s	264.40	Joback Method
dvisc	0.0061847	Pa×s	297.61	Joback Method
dvisc	0.0025955	Pa×s	330.83	Joback Method
dvisc	0.0012763	Pa×s	364.05	Joback Method
dvisc	0.0007067	Pa×s	397.26	Joback Method
dvisc	0.0004286	Pa×s	430.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	3.30	NIST Webbook

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=C624760&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

ie:	Ionization energy
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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