3-Ethoxypropanal

Other names: Propanal, 3-ethoxy
3-ethoxypropionaldehyde
Inchi: InChI=1S/C5H10O2/c1-2-7-5-3-4-6/h4H,2-3,5H2,1H3
InchiKey: RKSGQXSDRYHVTM-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: CCOCCC=O
Mol. weight [g/mol]: 102.13
CAS: 2806-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-213.30	kJ/mol	Joback Method
hf	-364.33	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	35.85	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.612		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
ripol	1175.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1185.00		NIST Webbook
tb	384.88	K	Joback Method
tc	558.32	K	Joback Method
tf	210.34	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.62	J/mol×K	384.88	Joback Method

cpg	173.77	J/mol×K	413.79	Joback Method
cpg	181.68	J/mol×K	442.69	Joback Method
cpg	189.36	J/mol×K	471.60	Joback Method
cpg	196.81	J/mol×K	500.50	Joback Method
cpg	204.01	J/mol×K	529.41	Joback Method
cpg	210.97	J/mol×K	558.32	Joback Method
dvisc	0.0030878	Pa×s	210.34	Joback Method
dvisc	0.0016395	Pa×s	239.43	Joback Method
dvisc	0.0009985	Pa×s	268.52	Joback Method
dvisc	0.0006700	Pa×s	297.61	Joback Method
dvisc	0.0004827	Pa×s	326.70	Joback Method
dvisc	0.0003669	Pa×s	355.79	Joback Method
dvisc	0.0002907	Pa×s	384.88	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2806851&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume