2-Butenoic acid, ethyl ester, (Z)-

Other names: Ethyl (Z)-2-butenoate
cis-Ethyl crotonate
Inchi: InChI=1S/C6H10O2/c1-3-5-6(7)8-4-2/h3,5H,4H2,1-2H3/b5-3-
InchiKey: ZFDIRQKJPRINOQ-HYXAFXHYSA-N
Formula: C6H10O2
SMILES: CC=CC(=O)OCC
Mol. weight [g/mol]: 114.14
CAS: 6776-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.06	kJ/mol	Joback Method
hf	-294.75	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook
tb	417.13	K	Joback Method
tc	603.73	K	Joback Method
tf	224.46	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.29	J/mol×K	417.13	Joback Method
cpg	227.98	J/mol×K	572.63	Joback Method
cpg	219.98	J/mol×K	541.53	Joback Method
cpg	211.61	J/mol×K	510.43	Joback Method
cpg	202.88	J/mol×K	479.33	Joback Method

cpg	193.78	J/mol×K	448.23	Joback Method
cpg	235.63	J/mol×K	603.73	Joback Method
dvisc	0.0002255	Pa×s	417.13	Joback Method
dvisc	0.0002879	Pa×s	385.02	Joback Method
dvisc	0.0003840	Pa×s	352.91	Joback Method
dvisc	0.0005428	Pa×s	320.80	Joback Method
dvisc	0.0008286	Pa×s	288.68	Joback Method
dvisc	0.0014062	Pa×s	256.57	Joback Method
dvisc	0.0027763	Pa×s	224.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6776198&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume