2-Octenoic acid, ethyl ester

Other names:	Ethyl 2-octenoate
	ethyl oct-2-enoate
Inchi:	InChI=1S/C10H18O2/c1-3-5-6-7-8-9-10(11)12-4-2/h8-9H,3-7H2,1-2H3/b9-8+
InchiKey:	AISZSTYLOVXFII-CMDGGOBGSA-N
Formula:	C10H18O2
SMILES:	CCCCCC=CC(=O)OCC
Mol. weight [g/mol]:	170.25
CAS:	2351-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-120.38	kJ/mol	Joback Method
hf	-377.31	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1231.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1557.00		NIST Webbook
tb	508.65	K	Joback Method
tc	688.43	K	Joback Method
tf	269.54	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.74	J/mol×K	508.65	Joback Method

cpg	414.10	J/mol×K	658.47	Joback Method
cpg	402.54	J/mol×K	628.50	Joback Method
cpg	390.44	J/mol×K	598.54	Joback Method
cpg	377.79	J/mol×K	568.58	Joback Method
cpg	364.56	J/mol×K	538.61	Joback Method
cpg	425.13	J/mol×K	688.43	Joback Method
dvisc	0.0001880	Pa×s	508.65	Joback Method
dvisc	0.0002455	Pa×s	468.80	Joback Method
dvisc	0.0003369	Pa×s	428.95	Joback Method
dvisc	0.0004933	Pa×s	389.10	Joback Method
dvisc	0.0007878	Pa×s	349.24	Joback Method
dvisc	0.0014196	Pa×s	309.39	Joback Method
dvisc	0.0030444	Pa×s	269.54	Joback Method

Sources

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=C2351908&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume