ETHYL 9-DECENOATE

Other names: Ethyl dec-9-enoate
9-Decenoic acid, ethyl ester
Inchi: InChI=1S/C12H22O2/c1-3-5-6-7-8-9-10-11-12(13)14-4-2/h3H,1,4-11H2,2H3
InchiKey: BKOJTZORTHALGP-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 198.31

Physical Properties

Property code	Value	Unit	Source
af	0.6320		Cheméo Relay (1.0)
gf	-95.92	kJ/mol	Joback Method
hf	-506.52	kJ/mol	Cheméo Relay (1.0)
hfus	28.34	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-3.79		Cheméo Relay (1.0)
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1387.80		NIST Webbook
rinpol	1389.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1711.00		NIST Webbook

ripol	1709.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1707.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1701.00		NIST Webbook
tb	507.29	K	Cheméo Relay (1.0)
tc	689.52	K	Cheméo Relay (1.0)
tf	247.25	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.34	J/mol×K	546.93	Joback Method
cpg	459.51	J/mol×K	575.71	Joback Method
cpg	474.05	J/mol×K	604.48	Joback Method

cpg	487.98	J/mol×K	633.26	Joback Method
cpg	501.31	J/mol×K	662.03	Joback Method
cpg	514.06	J/mol×K	690.81	Joback Method
cpg	526.24	J/mol×K	719.58	Joback Method
dvisc	0.0029144	Pa×s	295.40	Joback Method
dvisc	0.0013996	Pa×s	337.32	Joback Method
dvisc	0.0007904	Pa×s	379.24	Joback Method
dvisc	0.0005002	Pa×s	421.16	Joback Method
dvisc	0.0003439	Pa×s	463.09	Joback Method
dvisc	0.0002516	Pa×s	505.01	Joback Method
dvisc	0.0001931	Pa×s	546.93	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67233914&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
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