ETHYL TRANS-2-PENTENOATE

Other names: (E)-2-Pentenoic acid ethyl ester
Inchi: InChI=1S/C7H12O2/c1-3-5-6-7(8)9-4-2/h5-6H,3-4H2,1-2H3/b6-5+
InchiKey: AGMKVZDPATUSMS-AATRIKPKSA-N
Formula: C7H12O2
SMILES: CC/C=C/C(=O)OCC
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
af	0.4146		Cheméo Relay (1.0)
chl	-4020.00 ± 10.00	kJ/mol	NIST Webbook
gf	-145.64	kJ/mol	Joback Method
hf	-394.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-442.00 ± 3.00	kJ/mol	NIST Webbook
hfus	16.88	kJ/mol	Joback Method
hvap	48.00 ± 1.00	kJ/mol	NIST Webbook
hvap	48.00	kJ/mol	NIST Webbook
ie	9.71	eV	Cheméo Relay (1.0)
log10ws	-2.24		Cheméo Relay (1.0)
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	410.18	K	Cheméo Relay (1.0)
tc	602.92	K	Cheméo Relay (1.0)
tf	202.49	K	Cheméo Relay (1.0)
vc	0.413	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
cpg	233.44	J/mol×K	470.85	Joback Method
cpg	243.76	J/mol×K	501.68	Joback Method

cpg	253.64	J/mol×K	532.52	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	222.68	J/mol×K	440.01	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0029377	Pa×s	235.73	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0002208	Pa×s	440.01	Joback Method
hvapt	39.00	kJ/mol	293.00	NIST Webbook

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=C24410842&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
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume