ETHYL 2-NONYNOATE

Other names: Ethyl 2-nonynoate
ethyl non-2-ynoate
Ethyl octyne carbonate
Inchi: InChI=1S/C11H18O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h3-8H2,1-2H3
InchiKey: BFZNMUGAZYAMTG-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CCCCCCC#CC(=O)OCC
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
chl	-6494.80	kJ/mol	NIST Webbook
hf	-316.04	kJ/mol	Cheméo Relay (1.0)
hfl	-406.30 ± 6.00	kJ/mol	NIST Webbook
hfl	464.00	kJ/mol	NIST Webbook
hfus	30.16	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.523		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	501.44	K	Cheméo Relay (1.0)
tc	659.66	K	Cheméo Relay (1.0)
tf	238.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.50	J/mol×K	536.37	Joback Method
cpg	394.84	J/mol×K	568.23	Joback Method
cpg	408.58	J/mol×K	600.10	Joback Method
cpg	421.74	J/mol×K	631.96	Joback Method
cpg	434.31	J/mol×K	663.82	Joback Method

cpg	446.31	J/mol×K	695.69	Joback Method
cpg	457.74	J/mol×K	727.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10031922&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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