Ethyl 2-octynoate

Other names:	Ethyl 2-octynate
	Ethyl heptyne carboxylate
	2-Octynoic acid, ethyl ester
	ethyl oct-2-ynoate
Inchi:	InChI=1S/C10H16O2/c1-3-5-6-7-8-9-10(11)12-4-2/h3-7H2,1-2H3
InchiKey:	QPMDWYXUSMRVKT-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CCCCCC#CC(=O)OCC
Mol. weight [g/mol]:	168.23
CAS:	10519-20-7

Physical Properties

Property code	Value	Unit	Source
chl	-5837.90	kJ/mol	NIST Webbook
gf	2.20	kJ/mol	Joback Method
hf	-222.23	kJ/mol	Joback Method
hfl	-383.80 ± 5.00	kJ/mol	NIST Webbook
hfl	435.60	kJ/mol	NIST Webbook
hfus	27.57	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.133		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	513.49	K	Joback Method
tc	707.09	K	Joback Method
tf	380.72	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.69	J/mol×K	513.49	Joback Method
cpg	348.11	J/mol×K	545.76	Joback Method

cpg	361.00	J/mol×K	578.02	Joback Method
cpg	373.34	J/mol×K	610.29	Joback Method
cpg	385.15	J/mol×K	642.55	Joback Method
cpg	396.44	J/mol×K	674.82	Joback Method
cpg	407.19	J/mol×K	707.09	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=C10519207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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