Ethyl 2-heptynoate

Other names: 2-Heptynoic acid, ethyl ester
ethyl hept-2-ynoate
Inchi: InChI=1S/C9H14O2/c1-3-5-6-7-8-9(10)11-4-2/h3-6H2,1-2H3
InchiKey: GDCQMGYMFGPMCX-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCCC#CC(=O)OCC
Mol. weight [g/mol]: 154.21
CAS: 16930-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-6.22	kJ/mol	Joback Method
hf	-201.59	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.743		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	490.61	K	Joback Method
tc	686.68	K	Joback Method
tf	369.45	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.83	J/mol×K	490.61	Joback Method
cpg	303.21	J/mol×K	523.29	Joback Method
cpg	315.11	J/mol×K	555.97	Joback Method
cpg	326.53	J/mol×K	588.64	Joback Method
cpg	337.47	J/mol×K	621.32	Joback Method
cpg	347.93	J/mol×K	654.00	Joback Method
cpg	357.92	J/mol×K	686.68	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=C16930953&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume