2-Pentynoic acid ethyl ester

Other names: Ethyl-2-pentynoate
ethyl pent-2-yn-1-oate
Inchi: InChI=1S/C7H10O2/c1-3-5-6-7(8)9-4-2/h3-4H2,1-2H3
InchiKey: XDPRPKSTFBPPHU-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CCC#CC(=O)OCC
Mol. weight [g/mol]: 126.15
CAS: 55314-57-3

Physical Properties

Property code	Value	Unit	Source
chl	-3881.90 ± 2.50	kJ/mol	NIST Webbook
gf	-23.06	kJ/mol	Joback Method
hf	-250.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-302.00 ± 2.00	kJ/mol	NIST Webbook
hfus	19.79	kJ/mol	Joback Method
hvap	41.00	kJ/mol	NIST Webbook
hvap	51.00 ± 1.00	kJ/mol	NIST Webbook
hvap	52.00	kJ/mol	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.963		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	444.85	K	Joback Method
tc	645.78	K	Joback Method
tf	346.91	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.40	J/mol×K	444.85	Joback Method
cpg	219.27	J/mol×K	478.34	Joback Method
cpg	228.80	J/mol×K	511.83	Joback Method

cpg	237.99	J/mol×K	545.31	Joback Method
cpg	246.82	J/mol×K	578.80	Joback Method
cpg	255.30	J/mol×K	612.29	Joback Method
cpg	263.43	J/mol×K	645.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C55314573&Units=SI

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