2-Octynoic acid

Other names:	2-Octyn-1-oic acid
	Propiolic acid, pentyl ester
	Propiolic acid, pentyl-
	m-Pentyl propiolate
	oct-2-ynoic acid
Inchi:	InChI=1S/C8H12O2/c1-2-3-4-5-6-7-8(9)10/h2-5H2,1H3,(H,9,10)
InchiKey:	BQDKCWCMDBMLEH-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CCCCCC#CC(=O)O
Mol. weight [g/mol]:	140.18
CAS:	5663-96-7

Physical Properties

Property code	Value	Unit	Source
chl	-4535.90	kJ/mol	NIST Webbook
gf	-46.46	kJ/mol	Joback Method
hf	-200.96	kJ/mol	Joback Method
hfl	367.00	kJ/mol	NIST Webbook
hfl	-327.20 ± 4.00	kJ/mol	NIST Webbook
hfus	25.29	kJ/mol	Joback Method
hvap	58.98	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.655		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	537.49	K	Joback Method
tc	726.10	K	Joback Method
tf	276.15 ± 2.00	K	NIST Webbook
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.36	J/mol×K	537.49	Joback Method

cpg	283.18	J/mol×K	568.92	Joback Method
cpg	292.56	J/mol×K	600.36	Joback Method
cpg	301.52	J/mol×K	631.79	Joback Method
cpg	310.05	J/mol×K	663.23	Joback Method
cpg	318.19	J/mol×K	694.66	Joback Method
cpg	325.93	J/mol×K	726.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.70	K	2.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57073e+01
Coeff. B	-4.89147e+03
Coeff. C	-8.83370e+01
Temperature range (K), min.	405.15
Temperature range (K), max.	559.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C5663967&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume