2-Octynoic acid, methyl ester

Other names:	Folione
	Methyl hept-1-yne-1-carboxylate
	Methyl 2-octynate
	Methyl 2-octynoate
	Methyl heptyne carbonate
	Methyl heptine carbonate
	Vert de violette, artificial
	Methyl 2-octinate
	Methyl pentylacetylenecarboxylate
	NSC 72098
	methyl oct-2-ynoate
Inchi:	InChI=1S/C9H14O2/c1-3-4-5-6-7-8-9(10)11-2/h3-6H2,1-2H3
InchiKey:	FRLZQXRXIKQFNS-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CCCCCC#CC(=O)OC
Mol. weight [g/mol]:	154.21
CAS:	111-12-6

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
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1210.00		NIST Webbook

tb	491.70	K	NIST Webbook
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
hvapt	64.50	kJ/mol	297.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.00	K	0.50	NIST Webbook
tbrp	380.20	K	2.70	NIST Webbook
tbrp	367.20	K	1.30	NIST Webbook

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=C111126&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume