Methyl-2-heptynoate

Other names:	2-Heptynoic acid, methyl ester
	methyl hept-2-ynoate
Inchi:	InChI=1S/C8H12O2/c1-3-4-5-6-7-8(9)10-2/h3-5H2,1-2H3
InchiKey:	IATZLNCRIIUXJM-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CCCCC#CC(=O)OC
Mol. weight [g/mol]:	140.18
CAS:	18937-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-14.64	kJ/mol	Joback Method
hf	-180.95	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	44.71	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.353		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	467.73	K	Joback Method
tc	666.26	K	Joback Method
tf	358.18	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.02	J/mol×K	467.73	Joback Method
cpg	260.23	J/mol×K	500.82	Joback Method
cpg	271.01	J/mol×K	533.91	Joback Method
cpg	281.38	J/mol×K	567.00	Joback Method
cpg	291.33	J/mol×K	600.08	Joback Method
cpg	300.87	J/mol×K	633.17	Joback Method
cpg	309.98	J/mol×K	666.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18937785&Units=SI
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

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