4-HEPTENOIC ACID, METHYL ESTER

Other names: Methyl 4-heptenoate
Inchi: InChI=1S/C8H14O2/c1-3-4-5-6-7-8(9)10-2/h4-5H,3,6-7H2,1-2H3
InchiKey: CVDVXDORDMZHRW-SNAWJCMRSA-N
Formula: C8H14O2
SMILES: CC/C=C/CCC(=O)OC
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
af	0.4049		Cheméo Relay (1.0)
hf	-412.33	kJ/mol	Cheméo Relay (1.0)
hfus	19.46	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-2.00		Cheméo Relay (1.0)
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
ripol	1323.00		NIST Webbook
ripol	1323.00		NIST Webbook
tb	428.72	K	Cheméo Relay (1.0)
tc	621.56	K	Cheméo Relay (1.0)
tf	191.04	K	Cheméo Relay (1.0)
vc	0.456	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.30	J/mol×K	462.89	Joback Method
cpg	327.49	J/mol×K	646.21	Joback Method
cpg	317.95	J/mol×K	615.66	Joback Method
cpg	307.96	J/mol×K	585.10	Joback Method
cpg	297.52	J/mol×K	554.55	Joback Method
cpg	286.60	J/mol×K	524.00	Joback Method

cpg	275.19	J/mol×K	493.44	Joback Method
dvisc	0.0005355	Pa×s	354.94	Joback Method
dvisc	0.0002123	Pa×s	462.89	Joback Method
dvisc	0.0002744	Pa×s	426.91	Joback Method
dvisc	0.0003717	Pa×s	390.93	Joback Method
dvisc	0.0030324	Pa×s	247.00	Joback Method
dvisc	0.0008378	Pa×s	318.96	Joback Method
dvisc	0.0014687	Pa×s	282.98	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6843932&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume