

6-Heptenoic acid, ethyl ester

Other names:	Ethyl 6-heptenoate
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-8-9(10)11-4-2/h3H,1,4-8H2,2H3
InchiKey:	FTJATNSAFIFEDU-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCCCC(=O)OCC
Mol. weight [g/mol]:	156.22
CAS:	25118-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-121.18	kJ/mol	Joback Method
hf	-348.46	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
ripol	1609.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	478.29	K	Joback Method
tc	655.34	K	Joback Method
tf	261.59	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.44	J/molxK	478.29	Joback Method
cpg	318.12	J/molxK	507.80	Joback Method
cpg	330.31	J/molxK	537.31	Joback Method
cpg	342.00	J/molxK	566.81	Joback Method
cpg	353.22	J/molxK	596.32	Joback Method
cpg	363.97	J/molxK	625.83	Joback Method

cpg	374.26	J/mol×K	655.34	Joback Method
dvisc	0.0030378	Paxs	261.59	Joback Method
dvisc	0.0015428	Paxs	297.71	Joback Method
dvisc	0.0009072	Paxs	333.82	Joback Method
dvisc	0.0005918	Paxs	369.94	Joback Method
dvisc	0.0004165	Paxs	406.06	Joback Method
dvisc	0.0003104	Paxs	442.17	Joback Method
dvisc	0.0002419	Paxs	478.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C25118234&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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