

2-Heptenoic acid

Other names:	Ethyl 2-heptenoate hept-2-enoic acid
Inchi:	InChI=1S/C7H12O2/c1-2-3-4-5-6-7(8)9/h5-6H,2-4H2,1H3,(H,8,9)/b6-5+
InchiKey:	YURNCBVQZBJDAJ-AATRIKPKSA-N
Formula:	C7H12O2
SMILES:	CCCCC=CC(=O)O
Mol. weight [g/mol]:	128.17
CAS:	18999-28-5

Physical Properties

Property code	Value	Unit	Source
gf	-177.46	kJ/mol	Joback Method
hf	-335.40	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.817		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	499.70	K	NIST Webbook
tc	687.17	K	Joback Method
tf	274.32	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.53	J/molxK	509.77	Joback Method
cpg	256.98	J/molxK	539.34	Joback Method
cpg	265.97	J/molxK	568.90	Joback Method
cpg	274.53	J/molxK	598.47	Joback Method
cpg	282.68	J/molxK	628.04	Joback Method
cpg	290.43	J/molxK	657.60	Joback Method
cpg	297.80	J/molxK	687.17	Joback Method

dvisc	0.0194127	Paxs	274.32	Joback Method
dvisc	0.0051430	Paxs	313.56	Joback Method
dvisc	0.0018309	Paxs	352.80	Joback Method
dvisc	0.0008015	Paxs	392.04	Joback Method
dvisc	0.0004078	Paxs	431.29	Joback Method
dvisc	0.0002322	Paxs	470.53	Joback Method
dvisc	0.0001442	Paxs	509.77	Joback Method

Sources

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=C18999285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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