

7-Hydroxyheptanoic acid

Inchi:	InChI=1S/C7H14O3/c8-6-4-2-1-3-5-7(9)10/h8H,1-6H2,(H,9,10)
InchiKey:	PNAJBOZYCFSQDJ-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	O=C(O)CCCCCO
Mol. weight [g/mol]:	146.18
CAS:	3710-42-7

Physical Properties

Property code	Value	Unit	Source
gf	-394.50	kJ/mol	Joback Method
hf	-604.85	kJ/mol	Joback Method
hfs	-808.00 ± 3.00	kJ/mol	NIST Webbook
hfus	23.66	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.014		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	597.79	K	Joback Method
tc	763.12	K	Joback Method
tf	340.22	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.22	J/mol×K	597.79	Joback Method
cpg	321.85	J/mol×K	625.34	Joback Method
cpg	330.12	J/mol×K	652.90	Joback Method
cpg	338.02	J/mol×K	680.45	Joback Method
cpg	345.58	J/mol×K	708.01	Joback Method
cpg	352.80	J/mol×K	735.56	Joback Method
cpg	359.68	J/mol×K	763.12	Joback Method
dvisc	0.0151009	Pa×s	340.22	Joback Method

dvisc	0.0032602	Pa×s	383.15	Joback Method
dvisc	0.0009586	Pa×s	426.08	Joback Method
dvisc	0.0003527	Pa×s	469.00	Joback Method
dvisc	0.0001534	Pa×s	511.93	Joback Method
dvisc	0.0000759	Pa×s	554.86	Joback Method
dvisc	0.0000416	Pa×s	597.79	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=C3710427&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
hfs:	Solid phase 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

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