2-Hexynoic acid

Other names: hex-2-ynoic acid
Inchi: InChI=1S/C6H8O2/c1-2-3-4-5-6(7)8/h2-3H2,1H3,(H,7,8)
InchiKey: AKYAUBWOTZJUBI-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CCCC#CC(=O)O
Mol. weight [g/mol]: 112.13
CAS: 764-33-0

Physical Properties

Property code	Value	Unit	Source
gf	-63.30	kJ/mol	Joback Method
hf	-159.68	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.874		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	491.73	K	Joback Method
tc	684.96	K	Joback Method
tf	374.23	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.13	J/mol×K	491.73	Joback Method
cpg	197.70	J/mol×K	523.93	Joback Method
cpg	204.95	J/mol×K	556.14	Joback Method
cpg	211.88	J/mol×K	588.34	Joback Method
cpg	218.49	J/mol×K	620.55	Joback Method
cpg	224.79	J/mol×K	652.75	Joback Method
cpg	230.79	J/mol×K	684.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57106e+01
Coeff. B	-4.97061e+03
Coeff. C	-9.10340e+01
Temperature range (K), min.	413.15
Temperature range (K), max.	569.15

Sources

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=C764330&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume