

5-Hexynoic acid

Inchi:	InChI=1S/C6H8O2/c1-2-3-4-5-6(7)8/h1H,3-5H2,(H,7,8)
InchiKey:	VPFMEXRVUOPYRG-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	C#CCCCC(=O)O
Mol. weight [g/mol]:	112.13
CAS:	53293-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-43.03	kJ/mol	Joback Method
hf	-140.08	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.874		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	472.85	K	Joback Method
tc	655.53	K	Joback Method
tf	315.10	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.65	J/mol×K	472.85	Joback Method
cpg	199.95	J/mol×K	503.30	Joback Method
cpg	206.90	J/mol×K	533.74	Joback Method
cpg	213.50	J/mol×K	564.19	Joback Method
cpg	219.79	J/mol×K	594.64	Joback Method
cpg	225.76	J/mol×K	625.08	Joback Method
cpg	231.43	J/mol×K	655.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.50 ± 1.50	K	0.03	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57053e+01
Coeff. B	-4.84556e+03
Coeff. C	-8.67730e+01
Temperature range (K), min.	401.15
Temperature range (K), max.	553.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C53293008&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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