5-methylhexanoic acid

Other names: Hexanoic acid, 5-methyl-
Inchi: InChI=1S/C7H14O2/c1-6(2)4-3-5-7(8)9/h6H,3-5H2,1-2H3,(H,8,9)
InchiKey: MHPUGCYGQWGLJL-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CC(C)CCCC(=O)O
Mol. weight [g/mol]: 130.18
CAS: 628-46-6

Physical Properties

Property code	Value	Unit	Source
gf	-260.12	kJ/mol	Joback Method
hf	-457.90	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.897		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
ripol	1914.00		NIST Webbook
tb	486.00 ± 6.00	K	NIST Webbook
tc	678.63	K	Joback Method
tf	264.40	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.80	J/mol×K	505.17	Joback Method
cpg	276.01	J/mol×K	534.08	Joback Method
cpg	285.78	J/mol×K	562.99	Joback Method
cpg	295.14	J/mol×K	591.90	Joback Method
cpg	304.09	J/mol×K	620.81	Joback Method
cpg	312.64	J/mol×K	649.72	Joback Method
cpg	320.81	J/mol×K	678.63	Joback Method

dvisc	0.0353274	Pa×s	264.40	Joback Method
dvisc	0.0080276	Pa×s	304.53	Joback Method
dvisc	0.0025758	Pa×s	344.66	Joback Method
dvisc	0.0010476	Pa×s	384.78	Joback Method
dvisc	0.0005050	Pa×s	424.91	Joback Method
dvisc	0.0002761	Pa×s	465.04	Joback Method
dvisc	0.0001662	Pa×s	505.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60019e+01
Coeff. B	-4.65437e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	373.32
Temperature range (K), max.	512.51

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=C628466&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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume