Pentanoic acid, 4-methyl-

Other names:	4,4-Dimethylbutanoic acid
	4-Methyl-n-valeric acid
	4-Methylpentanoic acid
	4-Methylvaleric acid
	ISO-CAPROIC ACID
	Isobutylacetic acid
	Isocaproic acid
	Isohexanoic acid
	Isohexoic acid
	NSC 4126
	Valeric acid, 4-methyl-
Inchi:	InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
InchiKey:	FGKJLKRYENPLQH-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(C)CCC(=O)O
Mol. weight [g/mol]:	116.16
CAS:	646-07-1

Physical Properties

Property code	Value	Unit	Source
gf	-268.54	kJ/mol	Joback Method
hf	-437.26	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.507		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	921.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1809.00		NIST Webbook

ripol	1800.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1803.00		NIST Webbook
tb	482.29	K	Joback Method
tc	657.19	K	Joback Method
tf	253.13	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.38	J/mol×K	657.19	Joback Method
cpg	266.02	J/mol×K	628.04	Joback Method
cpg	258.31	J/mol×K	598.89	Joback Method
cpg	250.24	J/mol×K	569.74	Joback Method
cpg	241.81	J/mol×K	540.59	Joback Method
cpg	233.01	J/mol×K	511.44	Joback Method
cpg	223.83	J/mol×K	482.29	Joback Method
dvisc	0.0437428	Pa×s	253.13	Joback Method
dvisc	0.0001967	Pa×s	482.29	Joback Method
dvisc	0.0003288	Pa×s	444.10	Joback Method
dvisc	0.0006050	Pa×s	405.90	Joback Method
dvisc	0.0012640	Pa×s	367.71	Joback Method
dvisc	0.0031323	Pa×s	329.52	Joback Method
dvisc	0.0098475	Pa×s	291.32	Joback Method
hvapt	91.70	kJ/mol	410.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37649e+01

Coeff. B	-2.66279e+03
Coeff. C	-1.80874e+02
Temperature range (K), min.	378.45
Temperature range (K), max.	495.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.31866e+03
Coeff. B	-6.70896e+04
Coeff. C	-1.95683e+02
Coeff. D	1.46843e-04
Temperature range (K), min.	339.15
Temperature range (K), max.	481.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646071&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=939
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume