Pentanoic acid, 4-methyl-, ethyl ester

Other names:	4-Methylvaleric acid, ethyl ester
	Ethyl 4-methylpentanoate
	Ethyl 4-methylvalerate
	Ethyl isocaproate
	Ethyl isohexanoate
	Valeric acid, 4-methyl-, ethyl ester
Inchi:	InChI=1S/C8H16O2/c1-4-10-8(9)6-5-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	OFQRUTMGVBMTFQ-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCOC(=O)CCC(C)C
Mol. weight [g/mol]:	144.21
CAS:	25415-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	951.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	943.00		NIST Webbook

rinpol	947.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	943.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1206.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1193.00		NIST Webbook
tb	458.29	K	Joback Method
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.57	J/mol×K	637.16	Joback Method
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method

cpg	338.23	J/mol×K	607.34	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
hvapt	45.40	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49867e+01
Coeff. B	-3.87351e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	325.92
Temperature range (K), max.	462.75

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25415672&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

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