Pentanoic acid, 2-methyl-, ethyl ester

Other names:	Ethyl 2-methylvalerate
	Ethyl «alpha»-methylvalerate
	Manzanate
	ethyl 2-methylpentanoate
Inchi:	InChI=1S/C8H16O2/c1-4-6-7(3)8(9)10-5-2/h7H,4-6H2,1-3H3
InchiKey:	HZPKNSYIDSNZKW-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(C)C(=O)OCC
Mol. weight [g/mol]:	144.21
CAS:	39255-32-8

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	940.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1152.00		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	338.23	J/mol×K	607.34	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	279.83	J/mol×K	458.29	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
hvapt	48.40	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography: https://www.doi.org/10.1016/j.jct.2015.02.015

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=C39255328&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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