Pentanoic acid 1-methylpropyl ester

Other names: sec-Butyl pentanoate
Pentanoic acid, 2-butyl ester
Inchi: InChI=1S/C9H18O2/c1-4-6-7-9(10)11-8(3)5-2/h8H,4-7H2,1-3H3
InchiKey: WKIZFWVLAYCRDF-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCC(=O)OC(C)CC
Mol. weight [g/mol]: 158.24
CAS: 23361-74-2

Physical Properties

Property code	Value	Unit	Source
chl	-5489.80 ± 1.70	kJ/mol	NIST Webbook
gf	-211.46	kJ/mol	Joback Method
hf	-573.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-624.00 ± 2.00	kJ/mol	NIST Webbook
hfus	18.33	kJ/mol	Joback Method
hvap	51.00	kJ/mol	NIST Webbook
hvap	51.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1019.00		NIST Webbook
ripol	1224.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method

cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method
hvapt	41.00	kJ/mol	293.00	NIST Webbook

Sources

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=C23361742&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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