Pentanoic acid, phenylmethyl ester

Other names:	Valeric acid, benzyl ester
	Benzyanyl
	Benzyl pentanoate
	Benzyl valerate
	Benzyl valerianate
	Benzyl N-valerate
	Phenylmethyl valerate
	Phenylmethyl pentanoate
	Phenylmethyl (benzyl) valerate
Inchi:	InChI=1S/C12H16O2/c1-2-3-9-12(13)14-10-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3
InchiKey:	YZJCDVRXBOPXSQ-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	10361-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-71.35	kJ/mol	Joback Method
hf	-299.28	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.920		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	1920.00		NIST Webbook

ripol	1894.00		NIST Webbook
tb	576.93	K	Joback Method
tc	782.93	K	Joback Method
tf	323.58	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/mol×K	576.93	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	449.76	J/mol×K	714.26	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	409.22	J/mol×K	611.26	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
dvisc	0.0001842	Pa×s	576.93	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0011633	Pa×s	365.81	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method

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=C10361394&Units=SI

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
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