Pentanoic acid, 2-phenylethyl ester

Other names:	Phenylethyl valerate
	Valeric acid, phenethyl ester
	2-Phenethyl pentanoate
	Valeric acid, 2-phenylethyl ester
	Phenylethyl N-valerate
	2-Phenylethyl pentanoate
	Phenethyl valerate
	Phenylethyl pentanoate
	NSC 404213
Inchi:	InChI=1S/C13H18O2/c1-2-3-9-13(14)15-11-10-12-7-5-4-6-8-12/h4-8H,2-3,9-11H2,1H3
InchiKey:	PDGPIBIURNPBSE-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	7460-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-62.93	kJ/mol	Joback Method
hf	-319.92	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.962		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2034.00		NIST Webbook
tb	599.81	K	Joback Method
tc	802.73	K	Joback Method
tf	334.85	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.32	J/mol×K	599.81	Joback Method
cpg	459.12	J/mol×K	633.63	Joback Method
cpg	474.04	J/mol×K	667.45	Joback Method
cpg	488.11	J/mol×K	701.27	Joback Method
cpg	501.35	J/mol×K	735.09	Joback Method
cpg	513.77	J/mol×K	768.91	Joback Method
cpg	525.42	J/mol×K	802.73	Joback Method
dvisc	0.0021584	Pa×s	334.85	Joback Method
dvisc	0.0011004	Pa×s	379.01	Joback Method
dvisc	0.0006457	Pa×s	423.17	Joback Method
dvisc	0.0004190	Pa×s	467.33	Joback Method
dvisc	0.0002930	Pa×s	511.49	Joback Method
dvisc	0.0002169	Pa×s	555.65	Joback Method
dvisc	0.0001678	Pa×s	599.81	Joback Method

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=C7460744&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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