Pentyl phenylacetate

Other names:	Amyl phenylacetate
	Benzeneacetic acid, pentyl ester
	Acetic acid, phenyl-, pentyl ester
	N-Amyl phenylacetate
	Phenylacetic acid, pentyl ester
Inchi:	InChI=1S/C13H18O2/c1-2-3-7-10-15-13(14)11-12-8-5-4-6-9-12/h4-6,8-9H,2-3,7,10-11H2
InchiKey:	LRVLBFSVAFUOGO-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	5137-52-0

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	1537.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1529.29		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1507.65		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2047.00		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

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=C5137520&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

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