Benzoic acid, pentyl ester

Other names:	amyl benzoate
	benzoic acid, amyl ester
	n-Amyl benzoate
	n-Pentyl benzoate
	pentyl benzoate
Inchi:	InChI=1S/C12H16O2/c1-2-3-7-10-14-12(13)11-8-5-4-6-9-11/h4-6,8-9H,2-3,7,10H2,1H3
InchiKey:	QKNZNUNCDJZTCH-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	2049-96-9

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	-3.39		Crippen Method
logp	3.034		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2190.00	kPa	Critical Point Measurements for n-Alkyl Benzoates (C8 to C13)
rinpol	1465.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1462.00		NIST Webbook

rinpol	1456.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1462.27		NIST Webbook
rinpol	1440.46		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1474.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	2017.00		NIST Webbook
tb	533.00 ± 4.00	K	NIST Webbook
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	409.22	J/mol×K	611.26	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method
cpg	449.76	J/mol×K	714.26	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method

dvisc	0.0011633	Pa×s	365.81	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0001842	Pa×s	576.93	Joback Method
hvapt	85.90	kJ/mol	443.50	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=C2049969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical Point Measurements for n-Alkyl Benzoates (C8 to C13):	https://www.doi.org/10.1021/je700049s

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

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