Benzoic acid, 2-phenylethyl ester

Other names:	Benzoic acid, phenethyl ester
	«beta»-Phenylethyl benzoate
	Benzylcarbinyl benzoate
	Phenethyl alcohol, benzoate
	Phenethyl benzoate
	Phenylethyl benzoate
	2-Phenylethyl benzoate
	«beta»-Phenethyl benzoate
	2-Fenylethylester kyseliny benzoove
Inchi:	InChI=1S/C15H14O2/c16-15(14-9-5-2-6-10-14)17-12-11-13-7-3-1-4-8-13/h1-10H,11-12H
InchiKey:	OSORMYZMWHVFOZ-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	O=C(OCCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	226.27
CAS:	94-47-3

Physical Properties

Property code	Value	Unit	Source
gf	66.32	kJ/mol	Joback Method
hf	-124.67	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.086		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1825.00		NIST Webbook

rinpol	1858.90		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1854.00		NIST Webbook
ripol	2652.00		NIST Webbook
ripol	2652.00		NIST Webbook
ripol	2682.00		NIST Webbook
ripol	2668.00		NIST Webbook
ripol	2654.00		NIST Webbook
ripol	2621.00		NIST Webbook
tb	672.25	K	Joback Method
tc	909.92	K	Joback Method
tf	383.81	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.75	J/mol×K	672.25	Joback Method
cpg	482.53	J/mol×K	711.86	Joback Method
cpg	497.08	J/mol×K	751.47	Joback Method
cpg	510.44	J/mol×K	791.09	Joback Method
cpg	522.68	J/mol×K	830.70	Joback Method
cpg	533.85	J/mol×K	870.31	Joback Method
cpg	544.01	J/mol×K	909.92	Joback Method
dvisc	0.0015219	Pa×s	383.81	Joback Method
dvisc	0.0008139	Pa×s	431.88	Joback Method
dvisc	0.0004934	Pa×s	479.96	Joback Method
dvisc	0.0003277	Pa×s	528.03	Joback Method
dvisc	0.0002330	Pa×s	576.10	Joback Method

dvisc	0.0001746	Pa×s	624.18	Joback Method
dvisc	0.0001364	Pa×s	672.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94473&Units=SI
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

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