Benzoic acid, 2-hydroxy-, phenylmethyl ester

Other names:	Salicylic acid, benzyl ester
	Benzyl o-hydroxybenzoate
	Benzyl salicylate
	Salicyclic acid benzyl ester
	benzyle salicylate
Inchi:	InChI=1S/C14H12O3/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-9,15H,10H2
InchiKey:	ZCTQGTTXIYCGGC-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	O=C(OCc1ccccc1)c1ccccc1O
Mol. weight [g/mol]:	228.24
CAS:	118-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.72	kJ/mol	Joback Method
hf	-281.34	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.749		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1869.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1872.00		NIST Webbook

rinpol	1899.00	NIST Webbook
rinpol	1898.00	NIST Webbook
rinpol	1898.00	NIST Webbook
rinpol	1900.00	NIST Webbook
rinpol	1860.00	NIST Webbook
rinpol	1909.00	NIST Webbook
rinpol	1862.00	NIST Webbook
rinpol	1872.00	NIST Webbook
rinpol	1863.00	NIST Webbook
rinpol	1857.00	NIST Webbook
rinpol	1866.00	NIST Webbook
rinpol	1863.00	NIST Webbook
rinpol	1903.00	NIST Webbook
rinpol	1857.00	NIST Webbook
rinpol	1877.40	NIST Webbook
rinpol	1827.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1836.00	NIST Webbook
rinpol	1827.00	NIST Webbook
rinpol	1857.00	NIST Webbook
rinpol	1827.00	NIST Webbook
rinpol	1826.00	NIST Webbook
rinpol	1864.00	NIST Webbook
rinpol	1863.00	NIST Webbook
rinpol	1840.00	NIST Webbook
rinpol	1828.00	NIST Webbook
rinpol	1886.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1824.00	NIST Webbook
rinpol	1861.00	NIST Webbook
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rinpol	1861.00	NIST Webbook
rinpol	1850.10	NIST Webbook
rinpol	1870.00	NIST Webbook
rinpol	1899.00	NIST Webbook
rinpol	1869.80	NIST Webbook
rinpol	1866.00	NIST Webbook
rinpol	1827.00	NIST Webbook
rinpol	1816.00	NIST Webbook
rinpol	1828.00	NIST Webbook
rinpol	1876.00	NIST Webbook

rinpol	1859.00		NIST Webbook
rinpol	1850.10		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1816.00		NIST Webbook
ripol	2796.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2767.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2737.00		NIST Webbook
ripol	2810.00		NIST Webbook
ripol	2804.00		NIST Webbook
ripol	2804.00		NIST Webbook
ripol	2796.00		NIST Webbook
ripol	2737.00		NIST Webbook
tb	729.99	K	Joback Method
tc	979.95	K	Joback Method
tf	295.15 ± 1.50	K	NIST Webbook
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.18	J/mol×K	979.95	Joback Method
cpg	464.36	J/mol×K	729.99	Joback Method
cpg	477.44	J/mol×K	771.65	Joback Method
cpg	489.51	J/mol×K	813.31	Joback Method
cpg	500.71	J/mol×K	854.97	Joback Method
cpg	511.14	J/mol×K	896.63	Joback Method
cpg	520.92	J/mol×K	938.29	Joback Method
dvisc	0.0000120	Pa×s	729.99	Joback Method
dvisc	0.0002882	Pa×s	484.26	Joback Method
dvisc	0.0001379	Pa×s	525.22	Joback Method
dvisc	0.0000734	Pa×s	566.17	Joback Method
dvisc	0.0000426	Pa×s	607.12	Joback Method
dvisc	0.0000264	Pa×s	648.08	Joback Method
dvisc	0.0000174	Pa×s	689.04	Joback Method
hvapt	78.70	kJ/mol	314.50	NIST Webbook

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=C118581&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
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