

Benzyl Benzoate

Other names:	Ascabin
	Ascabiol
	BENYLATE
	BENZYL ALCOHOL BENZOIC ESTER
	BENZYL BENZENECARBOXYLATE
	Benzoic acid, benzyl ester
	Benzoic acid, phenylmethyl ester
	Benzyl phenylformate
	Benzylester kyseliny benzoove
	Benzylets
	Colebenz
	NSC 8081
	Novoscabin
	Peruscabin
	Phenylmethyl (benzyl) ester
	Phenylmethyl benzoate
	Scabagen
	Scabanca
	Scabide
	Scabiozon
	Scabitox
	Scobenol
	Vanzoate
	Venzoate
	Venzonate
Inchi:	InChI=1S/C14H12O2/c15-14(13-9-5-2-6-10-13)16-11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey:	SESFYSPDFLNCH-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(OCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	212.24
CAS:	120-51-4

Physical Properties

Property code	Value	Unit	Source
gf	57.90	kJ/mol	Joback Method
hf	-104.03	kJ/mol	Joback Method

hfus	22.89	kJ/mol	Joback Method
hvap	60.47	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.044		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1736.20		NIST Webbook
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ripol	2655.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2655.00		NIST Webbook
tb	596.70	K	NIST Webbook
tb	596.20 ± 1.00	K	NIST Webbook
tb	596.50 ± 0.50	K	NIST Webbook
tc	892.14	K	Joback Method

tf	292.00 ± 0.30	K	NIST Webbook
tf	294.99 ± 0.20	K	NIST Webbook
tf	294.00	K	NIST Webbook
tf	292.60 ± 0.50	K	NIST Webbook
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.57	J/mol×K	892.14	Joback Method
cpg	431.27	J/mol×K	689.83	Joback Method
cpg	445.36	J/mol×K	730.29	Joback Method
cpg	458.28	J/mol×K	770.75	Joback Method
cpg	470.08	J/mol×K	811.21	Joback Method
cpg	480.83	J/mol×K	851.67	Joback Method
cpg	415.95	J/mol×K	649.37	Joback Method
dvisc	0.0016037	Pa×s	372.54	Joback Method
dvisc	0.0008710	Pa×s	418.68	Joback Method
dvisc	0.0005339	Pa×s	464.82	Joback Method
dvisc	0.0003576	Pa×s	510.96	Joback Method
dvisc	0.0002559	Pa×s	557.09	Joback Method
dvisc	0.0001512	Pa×s	649.37	Joback Method
dvisc	0.0001928	Pa×s	603.23	Joback Method
hfust	20.44	kJ/mol	293.10	NIST Webbook
hfust	20.44	kJ/mol	293.10	NIST Webbook
hvapt	59.70	kJ/mol	549.50	NIST Webbook
hvapt	77.70	kJ/mol	325.00	NIST Webbook
srf	0.04	N/m	353.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure
srf	0.04	N/m	373.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure
srf	0.04	N/m	393.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure

srf	0.03	N/m	413.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure	
srf	0.03	N/m	433.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure	
srf	0.03	N/m	453.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure	
srf	0.03	N/m	473.15	Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure	

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52484e+01
Coeff. B	-5.42518e+03
Coeff. C	-8.63370e+01
Temperature range (K), min.	448.96
Temperature range (K), max.	632.30

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	9.04348e+01
Coeff. B	-1.27055e+04
Coeff. C	-1.02137e+01
Coeff. D	2.09556e-06
Temperature range (K), min.	292.55
Temperature range (K), max.	820.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120514&Units=SI
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1155
Effect of Hydrotropes on the Solubility and Mass Transfer Coefficient of Benzyl Benzoate in Water:	https://www.doi.org/10.1021/je049756u
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1155.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure: Measuring Surface Tension of Liquids at High Temperature and Elevated Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.doi.org/10.1021/je700578f

Legend

cp_g:	Ideal gas heat capacity
dv_{isc}:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{fust}:	Enthalpy of fusion at a given temperature
h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log_{10ws}:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
ri_{pol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
s_r_f:	Surface Tension
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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