

Benzoic acid, 2-benzoyl-

Other names:	Benzoic acid, o-benzoyl- o-Benzoylbenzoic acid Benzophenone-2-carboxylic acid 2-Benzoylbenzoic acid 2-Carboxybenzophenone Benzophenone-2-carbonic acid 2-Benzoquinonecarboxylic acid o-Carboxybenzophenone NSC 6646
Inchi:	InChI=1S/C14H10O3/c15-13(10-6-2-1-3-7-10)11-8-4-5-9-12(11)14(16)17/h1-9H,(H,16,17)
InchiKey:	FGTYTUFKXYPTML-UHFFFAOYSA-N
Formula:	C14H10O3
SMILES:	O=C(O)c1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]:	226.23
CAS:	85-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-112.47	kJ/mol	Joback Method
hf	-248.09	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.616		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	534.20	K	NIST Webbook
tc	1010.00	K	Joback Method
tf	402.25 ± 0.20	K	NIST Webbook
tf	401.95 ± 0.30	K	NIST Webbook
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.21	J/mol×K	777.98	Joback Method
cpg	460.54	J/mol×K	816.65	Joback Method
cpg	469.96	J/mol×K	855.32	Joback Method
cpg	478.54	J/mol×K	893.99	Joback Method
cpg	486.33	J/mol×K	932.66	Joback Method
cpg	493.41	J/mol×K	971.33	Joback Method
cpg	499.82	J/mol×K	1010.00	Joback Method
dvisc	0.0009334	Pa×s	473.58	Joback Method
dvisc	0.0004245	Pa×s	524.31	Joback Method
dvisc	0.0002219	Pa×s	575.05	Joback Method
dvisc	0.0001288	Pa×s	625.78	Joback Method
dvisc	0.0000811	Pa×s	676.51	Joback Method
dvisc	0.0000545	Pa×s	727.25	Joback Method
dvisc	0.0000386	Pa×s	777.98	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=C85529&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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