2-Benzoylbenzoic acid

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

Physical Properties

Property code	Value	Unit	Source
af	0.7943		Cheméo Relay (1.0)
gf	-112.47	kJ/mol	Joback Method
hf	-325.92	kJ/mol	Cheméo Relay (1.0)
hfus	27.00	kJ/mol	Joback Method
hvap	115.55	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-3.06		Cheméo Relay (1.0)
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	935.25	K	Cheméo Relay (1.0)
tf	402.25 ± 0.20	K	NIST Webbook
tf	401.95 ± 0.30	K	NIST Webbook
vc	0.609	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85529&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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