

Carbonic acid, 2-biphenyl isobutyl ester

Other names:	2-Phenylphenol, isoBOC
Inchi:	InChI=1S/C17H18O3/c1-13(2)12-19-17(18)20-16-11-7-6-10-15(16)14-8-4-3-5-9-14/h3-11
InchiKey:	QWFZNDGQWHEJIV-UHFFFAOYSA-N
Formula:	C17H18O3
SMILES:	CC(C)COC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	270.32

Physical Properties

Property code	Value	Unit	Source
gf	-33.91	kJ/mol	Joback Method
hf	-314.92	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.525		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	744.97	K	Joback Method
tc	975.62	K	Joback Method
tf	426.10	K	Joback Method
vc	0.807	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.97	J/mol×K	744.97	Joback Method
cpg	615.03	J/mol×K	783.41	Joback Method
cpg	629.83	J/mol×K	821.85	Joback Method
cpg	643.39	J/mol×K	860.30	Joback Method
cpg	655.76	J/mol×K	898.74	Joback Method
cpg	666.96	J/mol×K	937.18	Joback Method
cpg	677.03	J/mol×K	975.62	Joback Method

dvisc	0.0009165	Paxs	426.10	Joback Method
dvisc	0.0004838	Paxs	479.25	Joback Method
dvisc	0.0002901	Paxs	532.39	Joback Method
dvisc	0.0001909	Paxs	585.54	Joback Method
dvisc	0.0001347	Paxs	638.68	Joback Method
dvisc	0.0001002	Paxs	691.83	Joback Method
dvisc	0.0000778	Paxs	744.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U331409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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