

Benzoic acid, 3-methyl-, 4-biphenyl ester

Inchi:	InChI=1S/C20H16O2/c1-15-6-5-9-18(14-15)20(21)22-19-12-10-17(11-13-19)16-7-3-2-4-8
InchiKey:	VYSBBHOJVYYBGX-UHFFFAOYSA-N
Formula:	C20H16O2
SMILES:	<chem>Cc1cccc(C(=O)Oc2ccc(-c3ccccc3)cc2)c1</chem>
Mol. weight [g/mol]:	288.34

Physical Properties

Property code	Value	Unit	Source
gf	201.57	kJ/mol	Joback Method
hf	-14.28	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	77.42	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	4.881		Crippen Method
mcvol	228.820	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinqol	2701.00		NIST Webbook
tb	823.29	K	Joback Method
tc	1081.36	K	Joback Method
tf	491.62	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.78	J/molxK	823.29	Joback Method
cpg	658.95	J/molxK	866.30	Joback Method
cpg	672.62	J/molxK	909.31	Joback Method
cpg	684.91	J/molxK	952.33	Joback Method
cpg	695.89	J/molxK	995.34	Joback Method
cpg	705.66	J/molxK	1038.35	Joback Method
cpg	714.31	J/molxK	1081.36	Joback Method
dvisc	0.0006411	Paxs	491.62	Joback Method
dvisc	0.0003788	Paxs	546.90	Joback Method

dvisc	0.0002465	Paxs	602.18	Joback Method
dvisc	0.0001724	Paxs	657.46	Joback Method
dvisc	0.0001275	Paxs	712.73	Joback Method
dvisc	0.0000984	Paxs	768.01	Joback Method
dvisc	0.0000787	Paxs	823.29	Joback Method

Sources

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=U355716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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