

4-Methylbenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C20H16O2/c1-15-7-9-18(10-8-15)20(21)22-19-13-11-17(12-14-19)16-5-3-2-4-6

InchiKey: JEKZVVFJHBMTPY-UHFFFAOYSA-N

Formula: C20H16O2

SMILES: Cc1ccc(C(=O)Oc2ccc(-c3ccccc3)cc2)cc1

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
rinpol	2721.00		NIST Webbook
tb	823.29	K	Joback Method
tc	1081.36	K	Joback Method
tf	491.62	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002465	Pa×s	602.18	Joback Method
dvisc	0.0001724	Pa×s	657.46	Joback Method
dvisc	0.0001275	Pa×s	712.73	Joback Method
dvisc	0.0000984	Pa×s	768.01	Joback Method
dvisc	0.0000787	Pa×s	823.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354159&Units=SI

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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