4-METHOXYDIPHENYLMETHANE

Other names: 1-Benzyl-4-methoxybenzene
4-Methoxydiphenylmethane
Anisole, p-benzyl-
p-Benzylanisole
p-Methoxydiphenylmethane
p-Methoxyphenylphenylmethane
Inchi: InChI=1S/C14H14O/c1-15-14-9-7-13(8-10-14)11-12-5-3-2-4-6-12/h2-10H,11H2,1H3
InchiKey: GQLYCRTUQGSDSM-UHFFFAOYSA-N
Formula: C14H14O
SMILES: COc1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]: 198.27

Physical Properties

Property code	Value	Unit	Source
af	0.5167		Cheméo Relay (1.0)
gf	177.19	kJ/mol	Joback Method
hf	35.98	kJ/mol	Cheméo Relay (1.0)
hfus	20.90	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-4.29		Cheméo Relay (1.0)
logp	3.286		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	588.78	K	Cheméo Relay (1.0)
tc	805.03	K	Cheméo Relay (1.0)
tf	297.10	K	Cheméo Relay (1.0)
vc	0.615	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.75	J/mol×K	600.48	Joback Method
cpg	482.36	J/mol×K	837.55	Joback Method

cpg	470.90	J/mol×K	798.04	Joback Method
cpg	458.45	J/mol×K	758.53	Joback Method
cpg	444.95	J/mol×K	719.01	Joback Method
cpg	430.37	J/mol×K	679.50	Joback Method
cpg	414.65	J/mol×K	639.99	Joback Method
dvisc	0.0003280	Pa×s	467.81	Joback Method
dvisc	0.0001424	Pa×s	600.48	Joback Method
dvisc	0.0001799	Pa×s	556.25	Joback Method
dvisc	0.0002367	Pa×s	512.03	Joback Method
dvisc	0.0014623	Pa×s	335.13	Joback Method
dvisc	0.0004865	Pa×s	423.58	Joback Method
dvisc	0.0007910	Pa×s	379.36	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C834140&Units=SI

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