Benzene, 1-methoxy-4-(2-phenylethyl)-

Other names: Anisole, p-phenethyl-
1-(4-Methoxyphenyl)-2-phenylethane
Inchi: InChI=1S/C15H16O/c1-16-15-11-9-14(10-12-15)8-7-13-5-3-2-4-6-13/h2-6,9-12H,7-8H2,1
InchiKey: AFPZIAQJQAQDAQ-UHFFFAOYSA-N
Formula: C15H16O
SMILES: COc1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]: 212.29
CAS: 14310-21-5

Physical Properties

Property code	Value	Unit	Source
gf	185.61	kJ/mol	Joback Method
hf	-23.56	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
ie	8.00 ± 10.00	eV	NIST Webbook
log10ws	-4.01		Crippen Method
logp	3.480		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	623.36	K	Joback Method
tc	855.63	K	Joback Method
tf	346.40	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.73	J/mol×K	623.36	Joback Method
cpg	465.17	J/mol×K	662.07	Joback Method
cpg	481.41	J/mol×K	700.78	Joback Method
cpg	496.49	J/mol×K	739.50	Joback Method
cpg	510.46	J/mol×K	778.21	Joback Method
cpg	523.38	J/mol×K	816.92	Joback Method

cpg	535.29	J/mol×K	855.63	Joback Method
dvisc	0.0014186	Pa×s	346.40	Joback Method
dvisc	0.0007544	Pa×s	392.56	Joback Method
dvisc	0.0004582	Pa×s	438.72	Joback Method
dvisc	0.0003060	Pa×s	484.88	Joback Method
dvisc	0.0002192	Pa×s	531.04	Joback Method
dvisc	0.0001656	Pa×s	577.20	Joback Method
dvisc	0.0001305	Pa×s	623.36	Joback Method

Sources

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=C14310215&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

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