Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-4-methoxy-

Inchi: InChI=1S/C13H18O/c1-10(13(2,3)4)11-6-8-12(14-5)9-7-11/h6-9H,1H2,2-5H3
InchiKey: CXJOZMQAIWJYLG-UHFFFAOYSA-N
Formula: C13H18O
SMILES: C=C(c1ccc(OC)cc1)C(C)(C)C
Mol. weight [g/mol]: 190.28
CAS: 22666-53-1

Physical Properties

Property code	Value	Unit	Source
affp	897.90	kJ/mol	NIST Webbook
basg	869.10	kJ/mol	NIST Webbook
gf	138.49	kJ/mol	Joback Method
hf	-111.92	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	47.99	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.755		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
tb	544.25	K	Joback Method
tc	760.60	K	Joback Method
tf	284.14	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.67	J/mol×K	544.25	Joback Method
cpg	421.31	J/mol×K	580.31	Joback Method
cpg	437.86	J/mol×K	616.37	Joback Method
cpg	453.37	J/mol×K	652.42	Joback Method
cpg	467.89	J/mol×K	688.48	Joback Method
cpg	481.47	J/mol×K	724.54	Joback Method
cpg	494.17	J/mol×K	760.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22666531&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume