5-methoxyhexa-1,3,5-trien-1-yl)benzene

Inchi: InChI=1S/C13H14O/c1-12(14-2)8-6-7-11-13-9-4-3-5-10-13/h3-11H,1H2,2H3/b8-6+,11-7+

InchiKey: ATOJVVOASPCZPV-JMFBPXTISA-N

Formula: C13H14O

SMILES: C=C(C=CC=Cc1ccccc1)OC

Mol. weight [g/mol]: 186.25

CAS: 104055-92-7

Physical Properties

Property code	Value	Unit	Source
gf	305.72	kJ/mol	Joback Method
hf	142.74	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.416		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1692.30		NIST Webbook
rinpol	1692.30		NIST Webbook
tb	550.82	K	Joback Method
tc	772.20	K	Joback Method
tf	259.04	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.18	J/mol×K	550.82	Joback Method
cpg	379.12	J/mol×K	587.72	Joback Method
cpg	393.98	J/mol×K	624.61	Joback Method
cpg	407.83	J/mol×K	661.51	Joback Method
cpg	420.75	J/mol×K	698.40	Joback Method
cpg	432.81	J/mol×K	735.30	Joback Method
cpg	444.06	J/mol×K	772.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104055927&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume