Benzene,1-methoxy-3-(3-phenylpropyl)-

Other names: 1-Phenyl-3-(3-methoxyphenyl)propane
Inchi: InChI=1S/C16H18O/c1-17-16-12-6-11-15(13-16)10-5-9-14-7-3-2-4-8-14/h2-4,6-8,11-13H
InchiKey: NKQJUHNXDRPZFM-UHFFFAOYSA-N
Formula: C16H18O
SMILES: COc1cccc(CCCc2ccccc2)c1
Mol. weight [g/mol]: 226.31
CAS: 67081-95-2

Physical Properties

Property code	Value	Unit	Source
gf	194.03	kJ/mol	Joback Method
hf	-44.20	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	58.83	kJ/mol	Joback Method
ie	8.20 ± 0.50	eV	NIST Webbook
log10ws	-4.43		Crippen Method
logp	3.870		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	646.24	K	Joback Method
tc	873.99	K	Joback Method
tf	357.67	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.17	J/mol×K	646.24	Joback Method
cpg	517.03	J/mol×K	684.20	Joback Method
cpg	533.68	J/mol×K	722.16	Joback Method
cpg	549.17	J/mol×K	760.12	Joback Method
cpg	563.53	J/mol×K	798.08	Joback Method
cpg	576.83	J/mol×K	836.03	Joback Method
cpg	589.11	J/mol×K	873.99	Joback Method

dvisc	0.0013617	Pa×s	357.67	Joback Method
dvisc	0.0007124	Pa×s	405.76	Joback Method
dvisc	0.0004276	Pa×s	453.86	Joback Method
dvisc	0.0002830	Pa×s	501.96	Joback Method
dvisc	0.0002014	Pa×s	550.05	Joback Method
dvisc	0.0001513	Pa×s	598.14	Joback Method
dvisc	0.0001186	Pa×s	646.24	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=C67081952&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