

Benzene, methoxymethyl-pentamethyl-

Inchi:	InChI=1S/C13H20O/c1-8-9(2)11(4)13(7-14-6)12(5)10(8)3/h7H2,1-6H3
InchiKey:	QQFRJMBCRUNMHT-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	COCc1c(C)c(C)c(C)c(C)c1C
Mol. weight [g/mol]:	192.30
CAS:	20145-50-0

Physical Properties

Property code	Value	Unit	Source
gf	17.84	kJ/mol	Joback Method
hf	-264.69	kJ/mol	Joback Method
hfus	22.71	kJ/mol	Joback Method
hvap	52.53	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.375		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
tb	570.84	K	Joback Method
tc	770.98	K	Joback Method
tf	347.52	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.07	J/molxK	570.84	Joback Method
cpg	436.86	J/molxK	604.20	Joback Method
cpg	452.00	J/molxK	637.55	Joback Method
cpg	466.51	J/molxK	670.91	Joback Method
cpg	480.37	J/molxK	704.27	Joback Method
cpg	493.59	J/molxK	737.62	Joback Method
cpg	506.16	J/molxK	770.98	Joback Method
dvisc	0.0007142	Paxs	347.52	Joback Method
dvisc	0.0004792	Paxs	384.74	Joback Method

dvisc	0.0003449	Paxs	421.96	Joback Method
dvisc	0.0002619	Paxs	459.18	Joback Method
dvisc	0.0002072	Paxs	496.40	Joback Method
dvisc	0.0001694	Paxs	533.62	Joback Method
dvisc	0.0001422	Paxs	570.84	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=C20145500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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