Benzene, 2-methoxy-1,3-dimethyl-

Other names: 2,6-Dimethylanisole
Inchi: InChI=1S/C9H12O/c1-7-5-4-6-8(2)9(7)10-3/h4-6H,1-3H3
InchiKey: GFNZJAUVJCGWLW-UHFFFAOYSA-N
Formula: C9H12O
SMILES: COc1c(C)cccc1C
Mol. weight [g/mol]: 136.19
CAS: 1004-66-6

Physical Properties

Property code	Value	Unit	Source
gf	13.05	kJ/mol	Joback Method
hf	-147.72	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	41.64	kJ/mol	Joback Method
ie	8.51	eV	NIST Webbook
ie	8.10 ± 0.02	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.312		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1078.00		NIST Webbook
tb	455.70	K	NIST Webbook
tc	672.88	K	Joback Method
tf	264.88	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	464.38	Joback Method

cpg	298.13	J/mol×K	638.13	Joback Method
cpg	287.55	J/mol×K	603.38	Joback Method
cpg	276.44	J/mol×K	568.63	Joback Method
cpg	264.78	J/mol×K	533.88	Joback Method
cpg	252.59	J/mol×K	499.13	Joback Method
cpg	308.18	J/mol×K	672.88	Joback Method
dvisc	0.0001853	Pa×s	464.38	Joback Method
dvisc	0.0002266	Pa×s	431.13	Joback Method
dvisc	0.0002865	Pa×s	397.88	Joback Method
dvisc	0.0003782	Pa×s	364.63	Joback Method
dvisc	0.0005277	Pa×s	331.38	Joback Method
dvisc	0.0007933	Pa×s	298.13	Joback Method
dvisc	0.0013208	Pa×s	264.88	Joback Method

Sources

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=C1004666&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume