2-(3-METHOXYPHENYL)ETHANOL

Other names: Phenethyl alcohol, m-methoxy-
m-Methoxyphenethyl alcohol
m-Methoxyphenylethanol
1-(2-Hydroxyethyl)-3-methoxybenzene
2-(3-Methoxyphenyl)ethanol
3-Methoxyphenethyl alcohol

Inchi: InChI=1S/C9H12O2/c1-11-9-4-2-3-8(7-9)5-6-10/h2-4,7,10H,5-6H2,1H3

InchiKey: UPPGEJSCUZMCMW-UHFFFAOYSA-N

Formula: C9H12O2

SMILES: COc1cccc(CCO)c1

Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
hf	-272.46	kJ/mol	Cheméo Relay (1.0)
hfus	17.99	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Cheméo Relay (1.0)
ie	8.37	eV	Cheméo Relay (1.0)
log10ws	-1.21		Cheméo Relay (1.0)
logp	1.230		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1235.00		NIST Webbook
tb	549.48	K	Cheméo Relay (1.0)
tc	751.59	K	Cheméo Relay (1.0)
tf	262.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.51	J/mol×K	551.58	Joback Method
cpg	300.67	J/mol×K	583.99	Joback Method
cpg	311.28	J/mol×K	616.40	Joback Method
cpg	321.36	J/mol×K	648.80	Joback Method

cpg	330.92	J/mol×K	681.21	Joback Method
cpg	339.96	J/mol×K	713.62	Joback Method
cpg	348.51	J/mol×K	746.03	Joback Method
dvisc	0.0055162	Pa×s	313.18	Joback Method
dvisc	0.0018885	Pa×s	352.91	Joback Method
dvisc	0.0008032	Pa×s	392.65	Joback Method
dvisc	0.0003997	Pa×s	432.38	Joback Method
dvisc	0.0002237	Pa×s	472.11	Joback Method
dvisc	0.0001370	Pa×s	511.85	Joback Method
dvisc	0.0000901	Pa×s	551.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5020417&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point