

Benzeneethanol, 2-methoxy-

Other names:	Phenethyl alcohol, o-methoxy- 2-Methoxyphenethyl alcohol
Inchi:	InChI=1S/C9H12O2/c1-11-9-5-3-2-4-8(9)6-7-10/h2-5,10H,6-7H2,1H3
InchiKey:	XLDRDNQLEMMNNH-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	COc1ccccc1CCO
Mol. weight [g/mol]:	152.19
CAS:	7417-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-114.14	kJ/mol	Joback Method
hf	-288.48	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.230		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
ripol	1645.00		NIST Webbook
tb	551.58	K	Joback Method
tc	746.03	K	Joback Method
tf	313.18	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.51	J/mol×K	551.58	Joback Method
cpg	339.96	J/mol×K	713.62	Joback Method
cpg	330.92	J/mol×K	681.21	Joback Method
cpg	321.36	J/mol×K	648.80	Joback Method
cpg	311.28	J/mol×K	616.40	Joback Method
cpg	300.67	J/mol×K	583.99	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	1.30	NIST Webbook

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=C7417187&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices

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

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