3-Methoxybenzylamine

Other names:	m-Methoxybenzylamine
	Benzenemethanamine, 3-methoxy-
	Benzylamine, m-methoxy-
Inchi:	InChI=1S/C8H11NO/c1-10-8-4-2-3-7(5-8)6-9/h2-5H,6,9H2,1H3
InchiKey:	GRRIMVWABNHKBX-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	COc1cccc(CN)c1
Mol. weight [g/mol]:	137.18
CAS:	5071-96-5

Physical Properties

Property code	Value	Unit	Source
gf	80.71	kJ/mol	Joback Method
hf	-81.82	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.154		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	509.05	K	Joback Method
tc	730.98	K	Joback Method
tf	324.35	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.29	J/mol×K	509.05	Joback Method
cpg	263.62	J/mol×K	546.04	Joback Method
cpg	275.28	J/mol×K	583.03	Joback Method
cpg	286.30	J/mol×K	620.01	Joback Method
cpg	296.69	J/mol×K	657.00	Joback Method
cpg	306.45	J/mol×K	693.99	Joback Method

cpg	315.60	J/mol×K	730.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	4.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5071965&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
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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