3-METHOXYPHENETHYLAMINE

Other names:	2-(3-Methoxyphenyl)ethanamine
	2-(3-Methoxyphenyl)ethylamine
	3-Methoxy-«beta»-phenethylamine
	3-Methoxyphenylethylamine
	Benzeneethanamine, 3-methoxy-
	NSC 124706
	Phenethylamine, m-methoxy-
	m-Methoxyphenethylamine
	m-Methoxyphenylethylamine
Inchi:	InChI=1S/C9H13NO/c1-11-9-4-2-3-8(7-9)5-6-10/h2-4,7H,5-6,10H2,1H3
InchiKey:	WJBMRZAHTUFBGE-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	COc1cccc(CCN)c1
Mol. weight [g/mol]:	151.21

Physical Properties

Property code	Value	Unit	Source
hf	-88.47	kJ/mol	Cheméo Relay (1.0)
hfus	19.10	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	1.196		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
tb	522.38	K	Cheméo Relay (1.0)
tc	723.95	K	Cheméo Relay (1.0)
tf	303.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.02	J/mol×K	531.93	Joback Method
cpg	308.41	J/mol×K	568.29	Joback Method
cpg	321.08	J/mol×K	604.65	Joback Method

cpg	333.04	J/mol×K	641.01	Joback Method
cpg	344.32	J/mol×K	677.37	Joback Method
cpg	354.92	J/mol×K	713.73	Joback Method
cpg	364.86	J/mol×K	750.09	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039670&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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