

2,3-DIMETHOXYBENZYLAMINE

Other names:	2,3-Dimethoxybenzylamine
Inchi:	InChI=1S/C9H13NO2/c1-11-8-5-3-4-7(6-10)9(8)12-2/h3-5H,6,10H2,1-2H3
InchiKey:	LVMPWFJVYMXSNY-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	COc1cccc(CN)c1OC
Mol. weight [g/mol]:	167.21

Physical Properties

Property code	Value	Unit	Source
hfus	19.90	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-1.02		Cheméo Relay (1.0)
logp	1.163		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
tb	539.09	K	Cheméo Relay (1.0)
tf	309.06	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.11	J/mol×K	559.33	Joback Method
cpg	330.99	J/mol×K	595.46	Joback Method
cpg	343.27	J/mol×K	631.58	Joback Method
cpg	354.93	J/mol×K	667.71	Joback Method
cpg	365.96	J/mol×K	703.83	Joback Method
cpg	376.37	J/mol×K	739.96	Joback Method
cpg	386.14	J/mol×K	776.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	1.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4393093&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
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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