

3-Methoxy-4-methylaniline

Inchi:	InChI=1S/C8H11NO/c1-6-3-4-7(9)5-8(6)10-2/h3-5H,9H2,1-2H3
InchiKey:	ONADZNBSLRAJFW-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	COc1cc(N)ccc1C
Mol. weight [g/mol]:	137.18
CAS:	16452-01-0

Physical Properties

Property code	Value	Unit	Source
hf	-99.53	kJ/mol	Cheméo Relay (1.0)
hfus	16.12	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Cheméo Relay (1.0)
ie	7.48	eV	Cheméo Relay (1.0)
logp	1.586		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
tb	525.37	K	Cheméo Relay (1.0)
tc	732.35	K	Cheméo Relay (1.0)
tf	330.40	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	2.23000e+01
Coeff. B	5.64640e-01
Coeff. C	-2.40920e-04
Coeff. D	1.59000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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