

1,3-Benzodioxol-5-amine

Other names:	3,4-(Methylenedioxy)-aniline Aniline, 3,4-(methylenedioxy)- 1-Amino-3,4-dimethylenedioxybenzene 1-Amino-3,4-methylenedioxybenzene 4-Amino-1,2-methylenedioxybenzene 5-Amino-1,3-benzodioxole 5-Aminobenzodioxole 1,2-(Methylenedioxy)-4-aminobenzene NSC 155176
Inchi:	InChI=1S/C7H7NO2/c8-5-1-2-6-7(3-5)10-4-9-6/h1-3H,4,8H2
InchiKey:	XGNXYCFREOZBOL-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Nc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	137.14
CAS:	14268-66-7

Physical Properties

Property code	Value	Unit	Source
gf	63.88	kJ/mol	Joback Method
hf	-111.29	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	54.66	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.997		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	5198.13	kPa	Joback Method
tb	534.04	K	Joback Method
tc	778.02	K	Joback Method
tf	378.69	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	222.44	J/mol×K	534.04	Joback Method
cpg	232.83	J/mol×K	574.70	Joback Method
cpg	242.37	J/mol×K	615.37	Joback Method
cpg	251.14	J/mol×K	656.03	Joback Method
cpg	259.21	J/mol×K	696.69	Joback Method
cpg	266.64	J/mol×K	737.35	Joback Method
cpg	273.50	J/mol×K	778.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14268667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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