

Piperonylamine

Other names:	3,4-Methylenedioxybenzylamine 1,3-Benzodioxole-5-methanamine benzo-1,3-dioxole-5-methylamine
Inchi:	InChI=1S/C8H9NO2/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-3H,4-5,9H2
InchiKey:	ZILSBZLQGRBMOR-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	NCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	151.16
CAS:	2620-50-0

Physical Properties

Property code	Value	Unit	Source
gf	72.30	kJ/mol	Joback Method
hf	-131.93	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	0.874		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	556.92	K	Joback Method
tc	795.93	K	Joback Method
tf	389.96	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.57	J/molxK	556.92	Joback Method
cpg	277.04	J/molxK	596.76	Joback Method
cpg	287.63	J/molxK	636.59	Joback Method
cpg	297.42	J/molxK	676.43	Joback Method
cpg	306.46	J/molxK	716.26	Joback Method
cpg	314.83	J/molxK	756.10	Joback Method

cpg

322.61

J/mol×K

795.93

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2620500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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