Piperonylonitrile

Other names:	1,3-Benzodioxole-5-carbonitrile
	3,4-Methylene dioxy benzonitrile
	3,4-methylenedioxybenzonitrile
	5-Cyano-1,3-benzodioxole
	Benzonitrile, 3,4-methylenedioxy-
	benzo-1,3-dioxole-5-carbonitrile
Inchi:	InChI=1S/C8H5NO2/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-3H,5H2
InchiKey:	PKRWWZCDLJSJIF-UHFFFAOYSA-N
Formula:	C8H5NO2
SMILES:	N#Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	147.13
CAS:	4421-09-4

Physical Properties

Property code	Value	Unit	Source
gf	139.03	kJ/mol	Joback Method
hf	-0.84	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives
hvap	56.72	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.287		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	586.47	K	Joback Method
tc	833.00	K	Joback Method
tf	371.69	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	232.23	J/mol×K	586.47	Joback Method
cpg	241.07	J/mol×K	627.56	Joback Method
cpg	249.18	J/mol×K	668.65	Joback Method
cpg	256.62	J/mol×K	709.74	Joback Method
cpg	263.46	J/mol×K	750.82	Joback Method
cpg	269.77	J/mol×K	791.91	Joback Method
cpg	275.62	J/mol×K	833.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4421094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives:	https://www.doi.org/10.1021/je700035m
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume