3,4-Methylenedioxyphenylacetonitrile

Other names: 1,3-Benzodioxole-5-acetonitrile
Inchi: InChI=1S/C9H7NO2/c10-4-3-7-1-2-8-9(5-7)12-6-11-8/h1-2,5H,3,6H2
InchiKey: ZQPBOYASBNAXOZ-UHFFFAOYSA-N
Formula: C9H7NO2
SMILES: N#CCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 161.16
CAS: 4439-02-5

Physical Properties

Property code	Value	Unit	Source
gf	147.45	kJ/mol	Joback Method
hf	-21.48	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.481		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	609.35	K	Joback Method
tc	850.60	K	Joback Method
tf	382.96	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.72	J/mol×K	609.35	Joback Method
cpg	286.61	J/mol×K	649.56	Joback Method
cpg	295.72	J/mol×K	689.77	Joback Method
cpg	304.14	J/mol×K	729.97	Joback Method
cpg	311.92	J/mol×K	770.18	Joback Method
cpg	319.14	J/mol×K	810.39	Joback Method
cpg	325.86	J/mol×K	850.60	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4439025&Units=SI
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
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

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