

3,5-Dimethoxyphenylacetonitrile

Inchi:	InChI=1S/C10H11NO2/c1-12-9-5-8(3-4-11)6-10(7-9)13-2/h5-7H,3H2,1-2H3
InchiKey:	UUNRWZQWCNTSCV-UHFFFAOYSA-N
Formula:	C10H11NO2
SMILES:	COc1cc(CC#N)cc(OC)c1
Mol. weight [g/mol]:	177.20
CAS:	13388-75-5

Physical Properties

Property code	Value	Unit	Source
gf	49.65	kJ/mol	Joback Method
hf	-135.70	kJ/mol	Joback Method
hfus	18.80	kJ/mol	Joback Method
hvap	56.75	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.770		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	611.76	K	Joback Method
tc	831.48	K	Joback Method
tf	363.37	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.82	J/molxK	611.76	Joback Method
cpg	344.49	J/molxK	648.38	Joback Method
cpg	355.55	J/molxK	685.00	Joback Method
cpg	365.99	J/molxK	721.62	Joback Method
cpg	375.80	J/molxK	758.24	Joback Method
cpg	384.97	J/molxK	794.86	Joback Method
cpg	393.50	J/molxK	831.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13388755&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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