2,3-Dimethoxyphenylacetonitrile

Inchi: InChI=1S/C10H11NO2/c1-12-9-5-3-4-8(6-7-11)10(9)13-2/h3-5H,6H2,1-2H3
InchiKey: VAOKGCHIOACZHR-UHFFFAOYSA-N
Formula: C10H11NO2
SMILES: COc1cccc(CC#N)c1OC
Mol. weight [g/mol]: 177.20
CAS: 4468-57-9

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/mol×K	611.76	Joback Method
cpg	344.49	J/mol×K	648.38	Joback Method
cpg	355.55	J/mol×K	685.00	Joback Method
cpg	365.99	J/mol×K	721.62	Joback Method
cpg	375.80	J/mol×K	758.24	Joback Method
cpg	384.97	J/mol×K	794.86	Joback Method
cpg	393.50	J/mol×K	831.48	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=C4468579&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