

2,4,6-Trimethoxybenzonitrile

Other names:	Benzonitrile, 2,4,6-trimethoxy-
Inchi:	InChI=1S/C10H11NO3/c1-12-7-4-9(13-2)8(6-11)10(5-7)14-3/h4-5H,1-3H3
InchiKey:	GBRHJUMDNWLSCT-UHFFFAOYSA-N
Formula:	C10H11NO3
SMILES:	COc1cc(OC)c(C#N)c(OC)c1
Mol. weight [g/mol]:	193.20
CAS:	2571-54-2

Physical Properties

Property code	Value	Unit	Source
chs	-5150.00 ± 0.90	kJ/mol	NIST Webbook
gf	-64.98	kJ/mol	Joback Method
hf	-244.60 ± 2.60	kJ/mol	NIST Webbook
hfs	-357.20 ± 1.60	kJ/mol	NIST Webbook
hfus	19.60	kJ/mol	Joback Method
hsub	112.60 ± 2.00	kJ/mol	NIST Webbook
hsub	112.60 ± 2.00	kJ/mol	NIST Webbook
hvap	59.82	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.584		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	639.16	K	Joback Method
tc	857.09	K	Joback Method
tf	398.12	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.92	J/mol×K	639.16	Joback Method
cpg	366.33	J/mol×K	675.48	Joback Method
cpg	377.19	J/mol×K	711.80	Joback Method
cpg	387.45	J/mol×K	748.13	Joback Method

cpg	397.08	J/mol×K	784.45	Joback Method
cpg	406.05	J/mol×K	820.77	Joback Method
cpg	414.33	J/mol×K	857.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2571542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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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