

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

Physical Properties

Property code	Value	Unit	Source
hf	-232.16	kJ/mol	Cheméo Relay (1.0)
hfus	19.60	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-3.12		Cheméo Relay (1.0)
logp	1.584		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
tb	594.27	K	Cheméo Relay (1.0)
tf	384.87	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2571542&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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