

(S,S)-(+)-2,3-DIMETHOXY-1,4-BIS(DIMETHYLAMINO)BUTANE

Other names:	(S,S)-(+)-2,3-Dimethoxy-1,4-bis(dimethylamino)butane [S(R*,R*)]-2,3-dimethoxy-N,N,N',N'-tetramethylbutane-1,4-diamine
Inchi:	InChI=1S/C10H24N2O2/c1-11(2)7-9(13-5)10(14-6)8-12(3)4/h9-10H,7-8H2,1-6H3/t9-,10-
InchiKey:	VYQCQNCBTMHEFI-UWVGGRQHSA-N
Formula:	C10H24N2O2
SMILES:	CO[C@@H](CN(C)C)[C@H](CN(C)C)OC
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
hfus	23.03	kJ/mol	Joback Method
ie	7.57	eV	Cheméo Relay (1.0)
logp	0.140		Crippen Method
mcvol	183.460	ml/mol	McGowan Method
tb	493.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.35	J/mol×K	497.04	Joback Method
cpg	455.04	J/mol×K	524.76	Joback Method
cpg	471.10	J/mol×K	552.49	Joback Method
cpg	486.52	J/mol×K	580.21	Joback Method
cpg	501.32	J/mol×K	607.93	Joback Method
cpg	515.51	J/mol×K	635.65	Joback Method
cpg	529.09	J/mol×K	663.38	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C26549213&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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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