4-Bromo-2,5-dimethoxyphenethylamine

Other names:	Bromo-2,5-dimethoxyphenylethylamine
	2-CB
	BDMPEA
	2,5-Dimethoxy-4-bromophenethylamine
	Benzeneethanamine, 4-bromo-2,5-dimethoxy-
Inchi:	InChI=1S/C10H14BrNO2/c1-13-9-6-8(11)10(14-2)5-7(9)3-4-12/h5-6H,3-4,12H2,1-2H3
InchiKey:	YMHOBZXQZVXHBM-UHFFFAOYSA-N
Formula:	C10H14BrNO2
SMILES:	COc1cc(CCN)c(OC)cc1Br
Mol. weight [g/mol]:	260.13
CAS:	66142-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-12.39	kJ/mol	Joback Method
hf	-251.93	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	64.01	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	1.968		Crippen Method
mcvol	167.220	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	653.35	K	Joback Method
tc	879.36	K	Joback Method
tf	453.96	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.90	J/mol×K	653.35	Joback Method
cpg	413.53	J/mol×K	691.02	Joback Method

cpg	425.44	J/mol×K	728.69	Joback Method
cpg	436.62	J/mol×K	766.35	Joback Method
cpg	447.07	J/mol×K	804.02	Joback Method
cpg	456.80	J/mol×K	841.69	Joback Method
cpg	465.79	J/mol×K	879.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66142812&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume