

Brolamfetamine

Other names:	4-Bromo-2,5-dimethoxyamphetamine (.+/-)-2,5-Dimethoxy-4-bromoamphetamine DOB (.+/-)-4-Bromo-2,5-dimethoxy-«alpha»-methylphenethylamine 1-(4-Bromo-2,5-dimethoxyphenyl)-2-propanamine 2,5-Dimethoxy-4-bromoamphetamine
Inchi:	InChI=1S/C11H16BrNO2/c1-7(13)4-8-5-11(15-3)9(12)6-10(8)14-2/h5-7H,4,13H2,1-3H3
InchiKey:	FXMWUTGUCAKQQL-UHFFFAOYSA-N
Formula:	C11H16BrNO2
SMILES:	COc1cc(CC(C)N)c(OC)cc1Br
Mol. weight [g/mol]:	274.15
CAS:	64638-07-9

Physical Properties

Property code	Value	Unit	Source
gf	-6.41	kJ/mol	Joback Method
hf	-277.85	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
ie	7.94 ± 0.06	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
ie	7.94	eV	NIST Webbook
log10ws	-3.64		Crippen Method
logp	2.356		Crippen Method
mcvol	181.310	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	675.79	K	Joback Method
tc	902.07	K	Joback Method
tf	450.23	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	451.33	J/mol×K	675.79	Joback Method
cpg	464.96	J/mol×K	713.50	Joback Method
cpg	477.76	J/mol×K	751.22	Joback Method
cpg	489.75	J/mol×K	788.93	Joback Method
cpg	500.91	J/mol×K	826.64	Joback Method
cpg	511.26	J/mol×K	864.36	Joback Method
cpg	520.80	J/mol×K	902.07	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=C64638079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
h vap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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