N-Methyl-1-(1,3-benzodioxol-5-yl)-2-butanamine

Other names:	MBDB
	2-Butanamine, 1-(3,4-methylenedioxyphenyl), N-methyl
	2-Methylamino-1-(3,4-methylenedioxyphenyl)butane
	(.+/-.)-MBDB
Inchi:	InChI=1S/C12H17NO2/c1-3-10(13-2)6-9-4-5-11-12(7-9)15-8-14-11/h4-5,7,10,13H,3,6,8H
InchiKey:	USWVWJSAJAEEHQ-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	CCC(Cc1ccc2c(c1)OCO2)NC
Mol. weight [g/mol]:	207.27
CAS:	135795-90-3

Physical Properties

Property code	Value	Unit	Source
gf	126.48	kJ/mol	Joback Method
hf	-200.09	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.956		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1654.50		NIST Webbook
rinpol	1654.50		NIST Webbook
tb	625.64	K	Joback Method
tc	843.18	K	Joback Method
tf	389.44	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.14	J/mol×K	625.64	Joback Method
cpg	460.34	J/mol×K	661.90	Joback Method
cpg	474.55	J/mol×K	698.15	Joback Method

cpg	487.84	J/mol×K	734.41	Joback Method
cpg	500.28	J/mol×K	770.66	Joback Method
cpg	511.93	J/mol×K	806.92	Joback Method
cpg	522.85	J/mol×K	843.18	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=C135795903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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