1-(8-Bromo-2,3,6,7-tetrahydrodibenzo[1,2-b;4,5-b']difuran-4-yl-2-aminopropane, N-methyl

Inchi: InChI=1S/C14H18BrNO2/c1-8(16-2)7-11-9-3-5-18-14(9)12(15)10-4-6-17-13(10)11/h8,16

InchiKey: PGDKTEUJVIBCDB-UHFFFAOYSA-N

Formula: C14H18BrNO2

SMILES: CNC(C)Cc1c2c(c(Br)c3c1OCC3)OCC2

Mol. weight [g/mol]: 312.20

Physical Properties

Property code	Value	Unit	Source
gf	197.21	kJ/mol	Joback Method
hf	-156.31	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.469		Crippen Method
mcvol	201.860	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	2204.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2204.00		NIST Webbook
tb	763.91	K	Joback Method
tc	1000.49	K	Joback Method
tf	531.52	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.32	J/mol×K	763.91	Joback Method
cpg	579.37	J/mol×K	803.34	Joback Method
cpg	592.59	J/mol×K	842.77	Joback Method
cpg	605.11	J/mol×K	882.20	Joback Method
cpg	617.06	J/mol×K	921.63	Joback Method
cpg	628.55	J/mol×K	961.06	Joback Method
cpg	639.71	J/mol×K	1000.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640496&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