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

Inchi: InChI=1S/C13H16BrNO2/c1-7(15)6-10-8-2-4-17-13(8)11(14)9-3-5-16-12(9)10/h7H,2-6,15

InchiKey: FKRREVSELFOLDT-UHFFFAOYSA-N

Formula: C13H16BrNO2

SMILES: CC(N)Cc1c2c(c(Br)c3c1OCC3)OCC2

Mol. weight [g/mol]: 298.18

Physical Properties

Property code	Value	Unit	Source
gf	165.85	kJ/mol	Joback Method
hf	-155.35	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.209		Crippen Method
mcvol	187.770	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	763.39	K	Joback Method
tc	1012.11	K	Joback Method
tf	550.85	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.95	J/mol×K	763.39	Joback Method
cpg	533.18	J/mol×K	804.84	Joback Method
cpg	545.61	J/mol×K	846.30	Joback Method
cpg	557.38	J/mol×K	887.75	Joback Method
cpg	568.64	J/mol×K	929.20	Joback Method
cpg	579.51	J/mol×K	970.66	Joback Method
cpg	590.15	J/mol×K	1012.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640481&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

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