2C-B-fly

Other names: 1-(8-Bromo-2,3,6,7-tetrahydrodibenzo[1,2-b; 4,5-b']difuran-4-yl-2-aminoethane
Inchi: InChI=1S/C12H14BrNO2/c13-10-9-3-6-15-11(9)7(1-4-14)8-2-5-16-12(8)10/h1-6,14H2
InchiKey: YZDFADGMVOSVIX-UHFFFAOYSA-N
Formula: C12H14BrNO2
SMILES: NCCc1c2c(c(Br)c3c1OCC3)OCC2
Mol. weight [g/mol]: 284.15
CAS: 178557-21-6

Physical Properties

Property code	Value	Unit	Source
gf	159.87	kJ/mol	Joback Method
hf	-129.43	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	1.820		Crippen Method
mcvol	173.680	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	740.95	K	Joback Method
tc	990.15	K	Joback Method
tf	554.58	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.21	J/mol×K	740.95	Joback Method
cpg	479.58	J/mol×K	782.48	Joback Method
cpg	491.18	J/mol×K	824.02	Joback Method
cpg	502.15	J/mol×K	865.55	Joback Method
cpg	512.62	J/mol×K	907.08	Joback Method

cpg	522.73	J/mol×K	948.62	Joback Method
cpg	532.61	J/mol×K	990.15	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=C178557216&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