3-[4-(4-Aminobenzyl)anilino]-2-benzofuran-1(3h)-o

Inchi: InChI=1S/C21H18N2O2/c22-16-9-5-14(6-10-16)13-15-7-11-17(12-8-15)23-20-18-3-1-2-4
InchiKey: OLSMFJRLHSJFQC-UHFFFAOYSA-N
Formula: C21H18N2O2
SMILES: Nc1ccc(Cc2ccc(NC3OC(=O)c4ccccc43)cc2)cc1
Mol. weight [g/mol]: 330.38
CAS: 110194-18-8

Physical Properties

Property code	Value	Unit	Source
gf	442.16	kJ/mol	Joback Method
hf	88.77	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.141		Crippen Method
mcvol	252.010	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	999.07	K	Joback Method
tc	1270.90	K	Joback Method
tf	691.90	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.02	J/mol×K	999.07	Joback Method
cpg	821.47	J/mol×K	1044.38	Joback Method
cpg	832.62	J/mol×K	1089.68	Joback Method
cpg	842.62	J/mol×K	1134.99	Joback Method
cpg	851.60	J/mol×K	1180.29	Joback Method
cpg	859.68	J/mol×K	1225.60	Joback Method
cpg	867.00	J/mol×K	1270.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110194188&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume