

Fluoren-9-ol, 2-amino-3-bromo-

Inchi:	InChI=1S/C13H10BrNO/c14-11-5-9-7-3-1-2-4-8(7)13(16)10(9)6-12(11)15/h1-6,13,16H,15
InchiKey:	UOKLBOQEDRSRDJ-UHFFFAOYSA-N
Formula:	C13H10BrNO
SMILES:	<chem>Nc1cc2c(cc1Br)-c1ccccc1C2O</chem>
Mol. weight [g/mol]:	276.13
CAS:	100397-98-6

Physical Properties

Property code	Value	Unit	Source
gf	273.78	kJ/mol	Joback Method
hf	108.54	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.093		Crippen Method
mcvol	169.000	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	799.19	K	Joback Method
tc	1042.23	K	Joback Method
tf	568.05	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.21	J/mol×K	799.19	Joback Method
cpg	446.77	J/mol×K	839.70	Joback Method
cpg	455.80	J/mol×K	880.20	Joback Method
cpg	464.44	J/mol×K	920.71	Joback Method
cpg	472.82	J/mol×K	961.22	Joback Method
cpg	481.04	J/mol×K	1001.72	Joback Method
cpg	489.24	J/mol×K	1042.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100397986&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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