3-Aminobiphenyl, TFA

Inchi: InChI=1S/C14H10F3NO/c15-14(16,17)13(19)18-12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H
InchiKey: HWOWNVQWIAMGRQ-UHFFFAOYSA-N
Formula: C14H10F3NO
SMILES: O=C(Nc1cccc(-c2ccccc2)c1)C(F)(F)F
Mol. weight [g/mol]: 265.23

Physical Properties

Property code	Value	Unit	Source
gf	-338.93	kJ/mol	Joback Method
hf	-526.89	kJ/mol	Joback Method
hfus	28.23	kJ/mol	Joback Method
hvap	61.41	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.854		Crippen Method
mcvol	177.460	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	314.90		NIST Webbook
rinpol	315.38		NIST Webbook
tb	676.68	K	Joback Method
tc	902.13	K	Joback Method
tf	419.68	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.39	J/mol×K	676.68	Joback Method
cpg	480.59	J/mol×K	714.26	Joback Method
cpg	492.66	J/mol×K	751.83	Joback Method
cpg	503.68	J/mol×K	789.41	Joback Method
cpg	513.74	J/mol×K	826.98	Joback Method
cpg	522.92	J/mol×K	864.56	Joback Method
cpg	531.32	J/mol×K	902.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537414&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