1-Amino-5,6,7,8-tetrahydronaphthalene, TFA

Other names: 5-Amino-1,2,3,4-tetrahydronaphthalene, TFA
Inchi: InChI=1S/C12H12F3NO/c13-12(14,15)11(17)16-10-7-3-5-8-4-1-2-6-9(8)10/h3,5,7H,1-2,4
InchiKey: CCTAJRYHHDWLPA-UHFFFAOYSA-N
Formula: C12H12F3NO
SMILES: O=C(Nc1cccc2c1CCCC2)C(F)(F)F
Mol. weight [g/mol]: 243.22

Physical Properties

Property code	Value	Unit	Source
gf	-421.45	kJ/mol	Joback Method
hf	-646.63	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.066		Crippen Method
mcvol	162.180	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	272.80		NIST Webbook
rinpol	272.80		NIST Webbook
tb	624.90	K	Joback Method
tc	838.51	K	Joback Method
tf	401.90	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.20	J/mol×K	624.90	Joback Method
cpg	445.28	J/mol×K	660.50	Joback Method
cpg	458.29	J/mol×K	696.10	Joback Method
cpg	470.31	J/mol×K	731.71	Joback Method
cpg	481.42	J/mol×K	767.31	Joback Method
cpg	491.70	J/mol×K	802.91	Joback Method
cpg	501.23	J/mol×K	838.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R125110&Units=SI

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