5-Aminoindan, TFA

Other names: 5-Aminoindane, TFA
Inchi: InChI=1S/C11H10F3NO/c12-11(13,14)10(16)15-9-5-4-7-2-1-3-8(7)6-9/h4-6H,1-3H2,(H,1
InchiKey: AWCMVCZKRRLBFY-UHFFFAOYSA-N
Formula: C11H10F3NO
SMILES: O=C(Nc1ccc2c(c1)CCC2)C(F)(F)F
Mol. weight [g/mol]: 229.20

Physical Properties

Property code	Value	Unit	Source
gf	-417.77	kJ/mol	Joback Method
hf	-619.83	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.676		Crippen Method
mcvol	148.090	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	262.67		NIST Webbook
rinpol	262.67		NIST Webbook
tb	597.75	K	Joback Method
tc	807.99	K	Joback Method
tf	394.15	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.38	J/mol×K	597.75	Joback Method
cpg	394.17	J/mol×K	632.79	Joback Method
cpg	405.96	J/mol×K	667.83	Joback Method
cpg	416.85	J/mol×K	702.87	Joback Method
cpg	426.91	J/mol×K	737.91	Joback Method
cpg	436.21	J/mol×K	772.95	Joback Method
cpg	444.85	J/mol×K	807.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R125556&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