3-Aminofluoranthene, TFA

Inchi: InChI=1S/C18H10F3NO/c19-18(20,21)17(23)22-15-9-8-13-11-5-2-1-4-10(11)12-6-3-7-14
InchiKey: JTVRLTHKXILOBG-UHFFFAOYSA-N
Formula: C18H10F3NO
SMILES: O=C(Nc1ccc2c3c(cccc13)-c1ccccc1-2)C(F)(F)F
Mol. weight [g/mol]: 313.27

Physical Properties

Property code	Value	Unit	Source
gf	-122.73	kJ/mol	Joback Method
hf	-341.17	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	4.988		Crippen Method
mcvol	203.500	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	404.24		NIST Webbook
rinpol	404.24		NIST Webbook
rinpol	404.78		NIST Webbook
tb	800.72	K	Joback Method
tc	1031.37	K	Joback Method
tf	567.76	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.35	J/mol×K	800.72	Joback Method
cpg	583.11	J/mol×K	839.16	Joback Method
cpg	593.32	J/mol×K	877.60	Joback Method
cpg	603.16	J/mol×K	916.05	Joback Method
cpg	612.83	J/mol×K	954.49	Joback Method
cpg	622.50	J/mol×K	992.93	Joback Method
cpg	632.37	J/mol×K	1031.37	Joback Method

Sources

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=R537429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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