1-Aminophenanthrene TFA

Inchi: InChI=1S/C16H10F3NO/c17-16(18,19)15(21)20-14-7-3-6-12-11-5-2-1-4-10(11)8-9-13(12
InchiKey: RINIEHZRJIGSRV-UHFFFAOYSA-N
Formula: C16H10F3NO
SMILES: O=C(Nc1cccc2c1ccc1ccccc12)C(F)(F)F
Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-230.83	kJ/mol	Joback Method
hf	-434.03	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	67.53	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.494		Crippen Method
mcvol	190.480	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	366.92		NIST Webbook
rinpol	366.92		NIST Webbook
rinpol	366.20		NIST Webbook
tb	738.70	K	Joback Method
tc	966.83	K	Joback Method
tf	493.72	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.97	J/mol×K	738.70	Joback Method
cpg	532.68	J/mol×K	776.72	Joback Method
cpg	543.46	J/mol×K	814.74	Joback Method
cpg	553.45	J/mol×K	852.76	Joback Method
cpg	562.79	J/mol×K	890.79	Joback Method
cpg	571.61	J/mol×K	928.81	Joback Method
cpg	580.05	J/mol×K	966.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537390&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