2,4,6-TRIFLUOROANILINE

Other names: 2-Amino-1,3,5-trifluorobenzene
Benzenamine, 2,4,6-trifluoro-
Inchi: InChI=1S/C6H4F3N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2
InchiKey: BJSVKBGQDHUBHZ-UHFFFAOYSA-N
Formula: C6H4F3N
SMILES: Nc1c(F)cc(F)cc1F
Mol. weight [g/mol]: 147.10

Physical Properties

Property code	Value	Unit	Source
af	0.4416		Cheméo Relay (1.0)
hfus	18.61	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-1.93		Cheméo Relay (1.0)
logp	1.686		Crippen Method
mcvol	86.930	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	428.71	K	Cheméo Relay (1.0)
tc	653.40	K	Cheméo Relay (1.0)
tf	315.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.95	J/mol×K	448.64	Joback Method
cpg	182.53	J/mol×K	481.70	Joback Method
cpg	189.75	J/mol×K	514.77	Joback Method
cpg	196.60	J/mol×K	547.83	Joback Method
cpg	203.09	J/mol×K	580.89	Joback Method
cpg	209.25	J/mol×K	613.96	Joback Method
cpg	215.06	J/mol×K	647.02	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C363815&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point