2,3,4-TRIFLUOROANILINE

Inchi: InChI=1S/C6H4F3N/c7-3-1-2-4(10)6(9)5(3)8/h1-2H,10H2
InchiKey: WRDGNXCXTDDYBZ-UHFFFAOYSA-N
Formula: C6H4F3N
SMILES: Nc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 147.10

Physical Properties

Property code	Value	Unit	Source
af	0.4503		Cheméo Relay (1.0)
hfus	18.61	kJ/mol	Joback Method
hvap	53.70 ± 0.50	kJ/mol	NIST Webbook
ie	8.41	eV	Cheméo Relay (1.0)
logp	1.686		Crippen Method
mcvol	86.930	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	442.37	K	Cheméo Relay (1.0)
tc	648.71	K	Cheméo Relay (1.0)
vc	0.320	m3/kmol	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	6.40	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3862735&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

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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
vc: Critical Volume