ALPHA,ALPHA,ALPHA,6-TETRAFLUORO-M-TOLU

Other names: 3-Amino-4-fluorobenzotrifluoride
Alpha,alpha,alpha,6-tetrafluoro-m-toluidine
Inchi: InChI=1S/C7H5F4N/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3H,12H2
InchiKey: DRKWGMXFFCPZLW-UHFFFAOYSA-N
Formula: C7H5F4N
SMILES: Nc1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 179.12

Physical Properties

Property code	Value	Unit	Source
hf	-772.44	kJ/mol	Cheméo Relay (1.0)
hfus	17.25	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-2.15		Cheméo Relay (1.0)
logp	2.427		Crippen Method
mcvol	102.790	ml/mol	McGowan Method
tb	448.51	K	Cheméo Relay (1.0)
tf	329.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.78	J/mol×K	462.58	Joback Method
cpg	234.58	J/mol×K	495.39	Joback Method
cpg	243.72	J/mol×K	528.20	Joback Method
cpg	252.24	J/mol×K	561.01	Joback Method
cpg	260.15	J/mol×K	593.82	Joback Method
cpg	267.50	J/mol×K	626.63	Joback Method
cpg	274.32	J/mol×K	659.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.00	K	2.70	NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C535524&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point