4-Amino-3,5-dichlorobenzotrifluoride

Other names:	Benzenamine, 2,6-dichloro-4-(trifluoromethyl)- 4-amino-3,5-diklórbenzotrifluorid
Inchi:	InChI=1S/C7H4Cl2F3N/c8-4-1-3(7(10,11)12)2-5(9)6(4)13/h1-2H,13H2
InchiKey:	ITNMAZSPBLRJLU-UHFFFAOYSA-N
Formula:	C7H4Cl2F3N
SMILES:	Nc1c(Cl)cc(C(F)(F)F)cc1Cl
Mol. weight [g/mol]:	230.01
CAS:	24279-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-447.42	kJ/mol	Joback Method
hf	-580.46	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.594		Crippen Method
mcvol	125.500	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	543.15	K	Joback Method
tc	762.76	K	Joback Method
tf	379.92	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.91	J/mol×K	543.15	Joback Method
cpg	269.26	J/mol×K	579.75	Joback Method
cpg	276.96	J/mol×K	616.35	Joback Method
cpg	284.03	J/mol×K	652.95	Joback Method
cpg	290.52	J/mol×K	689.55	Joback Method
cpg	296.47	J/mol×K	726.15	Joback Method
cpg	301.92	J/mol×K	762.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24279398&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume