Benzenamine, 2-chloro-5-(trifluoromethyl)-

Other names:	m-Toluidine, 6-chloro-«alpha»,«alpha»,«alpha»-trifluoro-
	Azoene Fast Orange RD Salt
	C.I. 37050
	Daito Orange Salt RD
	Diazo Fast Orange RD
	Fast Orange RD Oil
	Fast Orange RD Salt
	Fast Orange Salt RDA
	Fast Orange Salt RDN
	Hiltosal Fast Orange RD Salt
	Orange Salt NRD
	Sanyo Fast Orange Salt RD
	2-Chloro-5-(trifluoromethyl)aniline
	3-Amino-4-chlorobenzotrifluoride
	4-Chloro-3-aminobenzotrifluoride
	6-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-m-toluidine
	Fast Orange Salt RD
	USAF MA-13
	3-Amino-4-chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	6-Chloro-3-(trifluoromethyl)aniline
	NSC 10318
Inchi:	InChI=1S/C7H5ClF3N/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3H,12H2
InchiKey:	VKTTYIXIDXWHKW-UHFFFAOYSA-N
Formula:	C7H5ClF3N
SMILES:	Nc1cc(C(F)(F)F)ccc1Cl
Mol. weight [g/mol]:	195.57
CAS:	121-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-425.86	kJ/mol	Joback Method
hf	-553.25	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	46.06	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.941		Crippen Method

mcvol	113.260	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	500.74	K	Joback Method
tc	714.25	K	Joback Method
tf	337.48	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	500.74	Joback Method
cpg	249.38	J/mol×K	536.33	Joback Method
cpg	258.20	J/mol×K	571.91	Joback Method
cpg	266.33	J/mol×K	607.50	Joback Method
cpg	273.82	J/mol×K	643.08	Joback Method
cpg	280.71	J/mol×K	678.67	Joback Method
cpg	287.04	J/mol×K	714.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.50 ± 0.50	K	1.00	NIST Webbook
tbrp	355.50 ± 0.50	K	1.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121506&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume