Benzenamine, 4-chloro-2-(trifluoromethyl)-

Other names:	o-Toluidine, 4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-
	C.I. Azoic Diazo Component 17
	C.I. 37055
	Diazo Fast Scarlet VD
	Fast Scarlet Salt VD
	Fast Scarlet VD Salt
	Scarlet Salt NVD
	4-Chloro-2-(trifluoromethyl)aniline
	2-Amino-5-chlorobenzotrifluoride
	5-Chloro-2-aminobenzotrifluoride
	2-Trifluoromethyl-4-chloroaniline
	4-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-o-toluidine
	5-Chloro-2-aminotrifluorotoluene
Inchi:	InChI=1S/C7H5ClF3N/c8-4-1-2-6(12)5(3-4)7(9,10)11/h1-3H,12H2
InchiKey:	CVINWVPRKDIGLL-UHFFFAOYSA-N
Formula:	C7H5ClF3N
SMILES:	Nc1ccc(Cl)cc1C(F)(F)F
Mol. weight [g/mol]:	195.57
CAS:	445-03-4

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	339.70	K	0.40	NIST Webbook
tbrp	350.00 ± 1.00	K	0.45	NIST Webbook
tbrp	360.50 ± 0.50	K	1.30	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=C445034&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