Benzenamine, 2-(trifluoromethoxy)-

Other names: 2-(trifluoromethoxy)aniline
Inchi: InChI=1S/C7H6F3NO/c8-7(9,10)12-6-4-2-1-3-5(6)11/h1-4H,11H2
InchiKey: ZFCOUBUSGHLCDT-UHFFFAOYSA-N
Formula: C7H6F3NO
SMILES: Nc1ccccc1OC(F)(F)F
Mol. weight [g/mol]: 177.12
CAS: 1535-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-509.30	kJ/mol	Joback Method
hf	-658.26	kJ/mol	Joback Method
hfus	15.75	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.167		Crippen Method
mcvol	106.890	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	480.75	K	Joback Method
tc	685.60	K	Joback Method
tf	317.27	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.96	J/mol×K	480.75	Joback Method
cpg	248.38	J/mol×K	514.89	Joback Method
cpg	258.12	J/mol×K	549.03	Joback Method
cpg	267.21	J/mol×K	583.18	Joback Method
cpg	275.66	J/mol×K	617.32	Joback Method
cpg	283.52	J/mol×K	651.46	Joback Method
cpg	290.81	J/mol×K	685.60	Joback Method

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=C1535757&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume