2-(Trifluoromethoxy)aniline

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]: 177.13

Physical Properties

Property code	Value	Unit	Source
hfus	15.75	kJ/mol	Joback Method
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	2.167		Crippen Method
mcvol	106.890	ml/mol	McGowan Method
tb	437.36	K	Cheméo Relay (1.0)
tf	218.65	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1535757&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point