2-(Trifluoromethyl)-1,4-phenyldiamine

Inchi: InChI=1S/C7H7F3N2/c8-7(9,10)5-3-4(11)1-2-6(5)12/h1-3H,11-12H2
InchiKey: ZQQOGBKIFPCFMJ-UHFFFAOYSA-N
Formula: C7H7F3N2
SMILES: Nc1ccc(N)c(C(F)(F)F)c1
Mol. weight [g/mol]: 176.14
CAS: 364-13-6

Physical Properties

Property code	Value	Unit	Source
gf	-347.48	kJ/mol	Joback Method
hf	-503.72	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	52.31	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.870		Crippen Method
mcvol	111.000	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	535.84	K	Joback Method
tc	754.42	K	Joback Method
tf	390.82	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.09	J/mol×K	535.84	Joback Method
cpg	276.26	J/mol×K	572.27	Joback Method
cpg	285.66	J/mol×K	608.70	Joback Method
cpg	294.34	J/mol×K	645.13	Joback Method
cpg	302.35	J/mol×K	681.56	Joback Method
cpg	309.72	J/mol×K	717.99	Joback Method
cpg	316.51	J/mol×K	754.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C364136&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

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

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