3-FLUOROBENZYLAMINE

Other names: Benzylamine, m-fluoro-
m-Fluorobenzylamine
3-Fluorobenzylamine
meta-Fluorobenzylamine
Inchi: InChI=1S/C7H8FN/c8-7-3-1-2-6(4-7)5-9/h1-4H,5,9H2
InchiKey: QVSVMNXRLWSNGS-UHFFFAOYSA-N
Formula: C7H8FN
SMILES: NCc1cccc(F)c1
Mol. weight [g/mol]: 125.15

Physical Properties

Property code	Value	Unit	Source
hf	-138.81	kJ/mol	Cheméo Relay (1.0)
hfus	15.81	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-0.82		Cheméo Relay (1.0)
logp	1.284		Crippen Method
mcvol	97.480	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
tb	442.95	K	Cheméo Relay (1.0)
tf	243.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.40	J/mol×K	463.02	Joback Method
cpg	207.17	J/mol×K	498.96	Joback Method
cpg	217.30	J/mol×K	534.90	Joback Method
cpg	226.82	J/mol×K	570.84	Joback Method
cpg	235.74	J/mol×K	606.77	Joback Method
cpg	244.11	J/mol×K	642.71	Joback Method
cpg	251.93	J/mol×K	678.65	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100823&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point