

Benzenemethanamine, 4-fluoro-

Other names:	Benzylamine, p-fluoro- 4-Fluorobenzylamine p-Fluorobenzylamine
Inchi:	InChI=1S/C7H8FN/c8-7-3-1-6(5-9)2-4-7/h1-4H,5,9H2
InchiKey:	IIFVWLUQBAIPMJ-UHFFFAOYSA-N
Formula:	C7H8FN
SMILES:	NCc1ccc(F)cc1
Mol. weight [g/mol]:	125.14
CAS:	140-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.52	kJ/mol	Joback Method
hf	-125.07	kJ/mol	Joback Method
hfus	15.81	kJ/mol	Joback Method
hvap	43.94	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.284		Crippen Method
mcvol	97.480	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinsol	996.20		NIST Webbook
tb	456.00	K	NIST Webbook
tb	456.20	K	NIST Webbook
tc	678.65	K	Joback Method
tf	291.44	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140750&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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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