

Benzenamine, 2,4-difluoro-

Other names:	Benzenamine, 2,4-difluoro- Aniline, 2,4-difluoro-
Inchi:	InChI=1S/C6H5F2N/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2
InchiKey:	CEPCPXLLFXPZGW-UHFFFAOYSA-N
Formula:	C6H5F2N
SMILES:	Nc1ccc(F)cc1F
Mol. weight [g/mol]:	129.11

Physical Properties

Property code	Value	Unit	Source
hfus	15.92	kJ/mol	Joback Method
hvap	52.10 ± 0.50	kJ/mol	NIST Webbook
ie	8.54	eV	NIST Webbook
logp	1.547		Crippen Method
mcvol	85.160	ml/mol	McGowan Method
tb	442.60	K	NIST Webbook
tf	294.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.45	J/mol×K	444.39	Joback Method
cpg	174.91	J/mol×K	479.08	Joback Method
cpg	182.90	J/mol×K	513.77	Joback Method
cpg	190.45	J/mol×K	548.47	Joback Method
cpg	197.56	J/mol×K	583.16	Joback Method
cpg	204.25	J/mol×K	617.85	Joback Method
cpg	210.54	J/mol×K	652.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	100.00	NIST Webbook

Sources

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=C367259&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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