

2,5-DIFLUOROBENZYLAMINE

Other names:	Benzenemethanamine, 2,5-difluoro-
Inchi:	InChI=1S/C7H7F2N/c8-6-1-2-7(9)5(3-6)4-10/h1-3H,4,10H2
InchiKey:	GDFBHCFIUBEQT-UHFFFAOYSA-N
Formula:	C7H7F2N
SMILES:	NCc1cc(F)ccc1F
Mol. weight [g/mol]:	143.14

Physical Properties

Property code	Value	Unit	Source
hfus	18.51	kJ/mol	Joback Method
hvap	56.33	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
logp	1.424		Crippen Method
mcvol	99.250	ml/mol	McGowan Method
tb	452.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.90	J/mol×K	467.27	Joback Method
cpg	214.68	J/mol×K	501.51	Joback Method
cpg	223.94	J/mol×K	535.76	Joback Method
cpg	232.68	J/mol×K	570.00	Joback Method
cpg	240.93	J/mol×K	604.24	Joback Method
cpg	248.71	J/mol×K	638.49	Joback Method
cpg	256.02	J/mol×K	672.73	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C85118065&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
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

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