

2-BROMO-4,6-DIFLUOROANILINE

Other names:	Benzenamine, 2-bromo-4,6-difluoro-
Inchi:	InChI=1S/C6H4BrF2N/c7-4-1-3(8)2-5(9)6(4)10/h1-2H,10H2
InchiKey:	WUJKFVGKLTWVSQ-UHFFFAOYSA-N
Formula:	C6H4BrF2N
SMILES:	Nc1c(F)cc(F)cc1Br
Mol. weight [g/mol]:	208.01

Physical Properties

Property code	Value	Unit	Source
af	0.4591		Cheméo Relay (1.0)
hf	-231.56	kJ/mol	Cheméo Relay (1.0)
hfus	20.81	kJ/mol	Joback Method
hvap	60.60	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-2.56		Cheméo Relay (1.0)
logp	2.310		Crippen Method
mcvol	102.660	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	484.15	K	Cheméo Relay (1.0)
tc	728.60	K	Cheméo Relay (1.0)
tf	325.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.91	J/mol×K	515.53	Joback Method
cpg	202.38	J/mol×K	553.25	Joback Method
cpg	209.38	J/mol×K	590.97	Joback Method
cpg	215.92	J/mol×K	628.68	Joback Method
cpg	222.02	J/mol×K	666.40	Joback Method
cpg	227.71	J/mol×K	704.12	Joback Method
cpg	233.00	J/mol×K	741.84	Joback Method

Sources

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=C444144&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

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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