2-Amino-6-fluorobenzylamine

Inchi: InChI=1S/C7H9FN2/c8-6-2-1-3-7(10)5(6)4-9/h1-3H,4,9-10H2
InchiKey: KBIXYFABFIYSAU-UHFFFAOYSA-N
Formula: C7H9FN2
SMILES: NCc1c(N)cccc1F
Mol. weight [g/mol]: 140.16
CAS: 175277-93-7

Physical Properties

Property code	Value	Unit	Source
gf	39.30	kJ/mol	Joback Method
hf	-102.75	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hvap	55.24	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	0.867		Crippen Method
mcvol	107.460	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	540.53	K	Joback Method
tc	768.19	K	Joback Method
tf	387.22	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.63	J/mol×K	540.53	Joback Method
cpg	256.16	J/mol×K	578.47	Joback Method
cpg	266.04	J/mol×K	616.42	Joback Method
cpg	275.29	J/mol×K	654.36	Joback Method
cpg	283.93	J/mol×K	692.30	Joback Method
cpg	292.00	J/mol×K	730.25	Joback Method
cpg	299.52	J/mol×K	768.19	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175277937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume