2,6-Difluorobenzylamine

Other names: Benzenemethanamine, 2,6-difluoro-
Inchi: InChI=1S/C7H7F2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H,4,10H2
InchiKey: PQCUDKMMPTXMAL-UHFFFAOYSA-N
Formula: C7H7F2N
SMILES: NCc1c(F)cccc1F
Mol. weight [g/mol]: 143.13
CAS: 69385-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-221.96	kJ/mol	Joback Method
hf	-332.65	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	43.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.424		Crippen Method
mcvol	99.250	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	467.27	K	Joback Method
tc	672.73	K	Joback Method
tf	304.55	K	Joback Method
vc	0.385	m3/kmol	Joback Method

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

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=C69385304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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