2,6-Difluorobenzamide

Other names: Benzamide, 2,6-difluoro-
Inchi: InChI=1S/C7H5F2NO/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H2,10,11)
InchiKey: AVRQBXVUUXHRMY-UHFFFAOYSA-N
Formula: C7H5F2NO
SMILES: NC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 157.12
CAS: 18063-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-350.88	kJ/mol	Joback Method
hf	-445.23	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	1.064		Crippen Method
mcvol	100.820	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	521.14	K	Joback Method
tc	736.51	K	Joback Method
tf	354.48	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.62	J/mol×K	521.14	Joback Method
cpg	225.43	J/mol×K	557.04	Joback Method
cpg	233.71	J/mol×K	592.93	Joback Method
cpg	241.46	J/mol×K	628.83	Joback Method
cpg	248.70	J/mol×K	664.72	Joback Method
cpg	255.46	J/mol×K	700.62	Joback Method
cpg	261.74	J/mol×K	736.51	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=C18063031&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
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
vc:	Critical Volume