2,5-Difluorobenzamide

Other names: 2,5-difluorobenzamide
Inchi: InChI=1S/C7H5F2NO/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H2,10,11)
InchiKey: BJKWHAILFUUIRT-UHFFFAOYSA-N
Formula: C7H5F2NO
SMILES: NC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 157.12

Physical Properties

Property code	Value	Unit	Source
hfus	20.11	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-2.19		Cheméo Relay (1.0)
logp	1.064		Crippen Method
mcvol	100.820	ml/mol	McGowan Method
tb	503.05	K	Cheméo Relay (1.0)

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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85118032&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature