

2,3-Difluorobenzamide

Inchi:	InChI=1S/C7H5F2NO/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3H,(H2,10,11)
InchiKey:	DDAINDMVKSETGF-UHFFFAOYSA-N
Formula:	C7H5F2NO
SMILES:	NC(=O)c1cccc(F)c1F
Mol. weight [g/mol]:	157.12
CAS:	18355-75-4

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
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/molxK	521.14	Joback Method
cpg	225.43	J/molxK	557.04	Joback Method
cpg	233.71	J/molxK	592.93	Joback Method
cpg	241.46	J/molxK	628.83	Joback Method
cpg	248.70	J/molxK	664.72	Joback Method
cpg	255.46	J/molxK	700.62	Joback Method
cpg	261.74	J/molxK	736.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18355754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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