

3,4-Difluorobenzamide, N-(4-methoxyphenyl)-

Inchi:	InChI=1S/C14H11F2NO2/c1-19-11-5-3-10(4-6-11)17-14(18)9-2-7-12(15)13(16)8-9/h2-8H
InchiKey:	ITUGFVHORJBPHY-UHFFFAOYSA-N
Formula:	C14H11F2NO2
SMILES:	COc1ccc(NC(=O)c2ccc(F)c(F)c2)cc1
Mol. weight [g/mol]:	263.24

Physical Properties

Property code	Value	Unit	Source
gf	-271.22	kJ/mol	Joback Method
hf	-477.19	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.226		Crippen Method
mcvol	181.560	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	2287.00		NIST Webbook
tb	713.02	K	Joback Method
tc	935.09	K	Joback Method
tf	463.94	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.91	J/molxK	713.02	Joback Method
cpg	491.65	J/molxK	750.03	Joback Method
cpg	503.43	J/molxK	787.04	Joback Method
cpg	514.28	J/molxK	824.05	Joback Method
cpg	524.23	J/molxK	861.06	Joback Method
cpg	533.30	J/molxK	898.08	Joback Method
cpg	541.52	J/molxK	935.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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