

Benzamide, N-(4-fluorophenyl)-2-methoxy-

Inchi:	InChI=1S/C14H12FNO2/c1-18-13-5-3-2-4-12(13)14(17)16-11-8-6-10(15)7-9-11/h2-9H,1H
InchiKey:	XWSMOGNYTBLKPT-UHFFFAOYSA-N
Formula:	C14H12FNO2
SMILES:	COC1CCCCC1C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]:	245.25

Physical Properties

Property code	Value	Unit	Source
gf	-66.78	kJ/mol	Joback Method
hf	-269.61	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.087		Crippen Method
mcvol	179.790	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	708.77	K	Joback Method
tc	939.76	K	Joback Method
tf	450.83	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.24	J/mol×K	708.77	Joback Method
cpg	485.76	J/mol×K	747.27	Joback Method
cpg	498.23	J/mol×K	785.77	Joback Method
cpg	509.67	J/mol×K	824.26	Joback Method
cpg	520.12	J/mol×K	862.76	Joback Method
cpg	529.63	J/mol×K	901.26	Joback Method
cpg	538.23	J/mol×K	939.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307057&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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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