Benzamide, 2-fluoro-N-(4-methoxyphenyl)-

Other names: Benzamide, N-(4-methoxyphenyl)-2-fluoro-
Inchi: InChI=1S/C14H12FNO2/c1-18-11-8-6-10(7-9-11)16-14(17)12-4-2-3-5-13(12)15/h2-9H,1H
InchiKey: HPAMAHNHZDHXKY-UHFFFAOYSA-N
Formula: C14H12FNO2
SMILES: COc1ccc(NC(=O)c2ccccc2F)cc1
Mol. weight [g/mol]: 245.25
CAS: 212209-96-6

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	2120.00		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

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=C212209966&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume