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

Physical Properties

Property code	Value	Unit	Source
hf	-333.65	kJ/mol	Cheméo Relay (1.0)
hfus	30.29	kJ/mol	Joback Method
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-4.18		Cheméo Relay (1.0)
logp	3.087		Crippen Method
mcvol	179.790	ml/mol	McGowan Method
tb	627.66	K	Cheméo Relay (1.0)
tf	413.77	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C212209966&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point