Benzamide, N-(2-iodo-4-methylphenyl)-2-fluoro-

Inchi: InChI=1S/C14H11FINO/c1-9-6-7-13(12(16)8-9)17-14(18)10-4-2-3-5-11(10)15/h2-8H,1H3

InchiKey: KXOHOUGEPPKILF-UHFFFAOYSA-N

Formula: C14H11FINO

SMILES: Cc1ccc(NC(=O)c2ccccc2F)c(I)c1

Mol. weight [g/mol]: 355.15

Physical Properties

Property code	Value	Unit	Source
gf	86.71	kJ/mol	Joback Method
hf	-71.99	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	3.991		Crippen Method
mcvol	199.740	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	784.47	K	Joback Method
tc	1042.85	K	Joback Method
tf	499.18	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.36	J/mol×K	784.47	Joback Method
cpg	500.13	J/mol×K	827.53	Joback Method
cpg	510.84	J/mol×K	870.60	Joback Method
cpg	520.59	J/mol×K	913.66	Joback Method
cpg	529.46	J/mol×K	956.72	Joback Method
cpg	537.54	J/mol×K	999.78	Joback Method
cpg	544.91	J/mol×K	1042.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307086&Units=SI

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