2,4,5-Trifluoro-3-methoxybenzamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C15H11F3INO2/c1-7-3-4-11(10(19)5-7)20-15(21)8-6-9(16)13(18)14(22-2)12(8

InchiKey: MOTKKLCEPPSGGG-UHFFFAOYSA-N

Formula: C15H11F3INO2

SMILES: COc1c(F)c(F)cc(C(=O)Nc2ccc(C)cc2I)c1F

Mol. weight [g/mol]: 421.15

Physical Properties

Property code	Value	Unit	Source
gf	-428.38	kJ/mol	Joback Method
hf	-651.48	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.278		Crippen Method
mcvol	223.240	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2637.00		NIST Webbook
tb	843.25	K	Joback Method
tc	1076.36	K	Joback Method
tf	571.42	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.17	J/mol×K	843.25	Joback Method
cpg	586.62	J/mol×K	882.10	Joback Method
cpg	596.13	J/mol×K	920.95	Joback Method
cpg	604.73	J/mol×K	959.81	Joback Method
cpg	612.44	J/mol×K	998.66	Joback Method
cpg	619.29	J/mol×K	1037.51	Joback Method
cpg	625.30	J/mol×K	1076.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358074&Units=SI
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

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