2-Fluoro-6-trifluoromethylbenzamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C15H10F4INO/c1-8-5-6-12(11(20)7-8)21-14(22)13-9(15(17,18)19)3-2-4-10(13)

InchiKey: CRFPHYUGKPPBKX-UHFFFAOYSA-N

Formula: C15H10F4INO

SMILES: Cc1ccc(NC(=O)c2c(F)cccc2C(F)(F)F)c(I)c1

Mol. weight [g/mol]: 423.14

Physical Properties

Property code	Value	Unit	Source
gf	-496.09	kJ/mol	Joback Method
hf	-701.18	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	74.17	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.010		Crippen Method
mcvol	219.140	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2424.00		NIST Webbook
tb	806.91	K	Joback Method
tc	1043.14	K	Joback Method
tf	527.16	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.65	J/mol×K	806.91	Joback Method
cpg	575.23	J/mol×K	846.28	Joback Method
cpg	584.91	J/mol×K	885.65	Joback Method
cpg	593.79	J/mol×K	925.02	Joback Method
cpg	601.96	J/mol×K	964.39	Joback Method
cpg	609.51	J/mol×K	1003.77	Joback Method
cpg	616.53	J/mol×K	1043.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358121&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