2,5-Difluorobenzamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C14H10F2INO/c1-8-2-5-13(12(17)6-8)18-14(19)10-7-9(15)3-4-11(10)16/h2-7H

InchiKey: ZTDDOIAVBBSXCE-UHFFFAOYSA-N

Formula: C14H10F2INO

SMILES: Cc1ccc(NC(=O)c2cc(F)ccc2F)c(I)c1

Mol. weight [g/mol]: 373.14

Physical Properties

Property code	Value	Unit	Source
gf	-117.73	kJ/mol	Joback Method
hf	-279.57	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	74.88	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.130		Crippen Method
mcvol	201.510	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	788.72	K	Joback Method
tc	1036.86	K	Joback Method
tf	512.29	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.37	J/mol×K	788.72	Joback Method
cpg	505.44	J/mol×K	830.08	Joback Method
cpg	515.55	J/mol×K	871.43	Joback Method
cpg	524.77	J/mol×K	912.79	Joback Method
cpg	533.17	J/mol×K	954.14	Joback Method
cpg	540.82	J/mol×K	995.50	Joback Method
cpg	547.78	J/mol×K	1036.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358052&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