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

Inchi: InChI=1S/C15H14INO/c1-10-7-8-14(13(16)9-10)17-15(18)12-6-4-3-5-11(12)2/h3-9H,1-2H

InchiKey: WYVYIEXNJANNTD-UHFFFAOYSA-N

Formula: C15H14INO

SMILES: Cc1ccc(NC(=O)c2ccccc2C)c(I)c1

Mol. weight [g/mol]: 351.18

Physical Properties

Property code	Value	Unit	Source
gf	289.94	kJ/mol	Joback Method
hf	103.48	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.160		Crippen Method
mcvol	212.060	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	808.08	K	Joback Method
tc	1072.07	K	Joback Method
tf	509.86	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.71	J/mol×K	808.08	Joback Method
cpg	546.58	J/mol×K	852.08	Joback Method
cpg	558.32	J/mol×K	896.08	Joback Method
cpg	569.02	J/mol×K	940.08	Joback Method
cpg	578.78	J/mol×K	984.07	Joback Method
cpg	587.70	J/mol×K	1028.07	Joback Method
cpg	595.86	J/mol×K	1072.07	Joback Method

Sources

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=U307009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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