Cyclopentanecarboxamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C13H16INO/c1-9-6-7-12(11(14)8-9)15-13(16)10-4-2-3-5-10/h6-8,10H,2-5H2,1H

InchiKey: LMOBJRHCFDRLDT-UHFFFAOYSA-N

Formula: C13H16INO

SMILES: Cc1ccc(NC(=O)C2CCCC2)c(I)c1

Mol. weight [g/mol]: 329.18

Physical Properties

Property code	Value	Unit	Source
gf	206.87	kJ/mol	Joback Method
hf	-19.82	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.728		Crippen Method
mcvol	196.780	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	745.94	K	Joback Method
tc	1005.97	K	Joback Method
tf	459.28	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.07	J/mol×K	745.94	Joback Method
cpg	525.49	J/mol×K	789.28	Joback Method
cpg	539.62	J/mol×K	832.62	Joback Method
cpg	552.54	J/mol×K	875.96	Joback Method
cpg	564.37	J/mol×K	919.30	Joback Method
cpg	575.18	J/mol×K	962.63	Joback Method
cpg	585.10	J/mol×K	1005.97	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=U307031&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