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

Inchi: InChI=1S/C14H18INO/c1-10-7-8-13(12(15)9-10)16-14(17)11-5-3-2-4-6-11/h7-9,11H,2-6H

InchiKey: QTDQOWUBHZMOQZ-UHFFFAOYSA-N

Formula: C14H18INO

SMILES: Cc1ccc(NC(=O)C2CCCCC2)c(I)c1

Mol. weight [g/mol]: 343.20

Physical Properties

Property code	Value	Unit	Source
gf	203.19	kJ/mol	Joback Method
hf	-46.62	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.118		Crippen Method
mcvol	210.870	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	2390.00		NIST Webbook
tb	773.09	K	Joback Method
tc	1035.07	K	Joback Method
tf	467.03	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.78	J/mol×K	773.09	Joback Method
cpg	583.17	J/mol×K	816.75	Joback Method
cpg	598.10	J/mol×K	860.42	Joback Method
cpg	611.67	J/mol×K	904.08	Joback Method
cpg	623.97	J/mol×K	947.74	Joback Method
cpg	635.09	J/mol×K	991.40	Joback Method
cpg	645.12	J/mol×K	1035.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306952&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