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

Inchi: InChI=1S/C12H14INO/c1-8-5-6-11(10(13)7-8)14-12(15)9-3-2-4-9/h5-7,9H,2-4H2,1H3,(H,
InchiKey: AOLMIWAXRMATOU-UHFFFAOYSA-N
Formula: C12H14INO
SMILES: Cc1ccc(NC(=O)C2CCC2)c(I)c1
Mol. weight [g/mol]: 315.15

Physical Properties

Property code	Value	Unit	Source
gf	210.55	kJ/mol	Joback Method
hf	6.98	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	68.55	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.338		Crippen Method
mcvol	182.690	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	718.79	K	Joback Method
tc	976.72	K	Joback Method
tf	451.53	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.17	J/mol×K	718.79	Joback Method
cpg	469.44	J/mol×K	761.78	Joback Method
cpg	482.55	J/mol×K	804.77	Joback Method
cpg	494.61	J/mol×K	847.75	Joback Method
cpg	505.73	J/mol×K	890.74	Joback Method
cpg	515.99	J/mol×K	933.73	Joback Method
cpg	525.52	J/mol×K	976.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307053&Units=SI

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