Propanamide, N-(2-iodo-4-methylphenyl)-2,2-dimethyl-

Inchi: InChI=1S/C12H16INO/c1-8-5-6-10(9(13)7-8)14-11(15)12(2,3)4/h5-7H,1-4H3,(H,14,15)
InchiKey: BGEQNDMAJXNQSN-UHFFFAOYSA-N
Formula: C12H16INO
SMILES: Cc1ccc(NC(=O)C(C)(C)C)c(I)c1
Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	164.74	kJ/mol	Joback Method
hf	-68.41	kJ/mol	Joback Method
hfus	23.79	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.584		Crippen Method
mcvol	193.550	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	704.55	K	Joback Method
tc	952.42	K	Joback Method
tf	439.53	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.05	J/mol×K	704.55	Joback Method
cpg	485.82	J/mol×K	745.86	Joback Method
cpg	498.51	J/mol×K	787.17	Joback Method
cpg	510.22	J/mol×K	828.49	Joback Method
cpg	521.04	J/mol×K	869.80	Joback Method
cpg	531.06	J/mol×K	911.11	Joback Method
cpg	540.38	J/mol×K	952.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307201&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

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