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

Inchi: InChI=1S/C11H14INO/c1-7(2)11(14)13-10-5-4-8(3)6-9(10)12/h4-7H,1-3H3,(H,13,14)
InchiKey: GHLXAEZLMCTMAY-UHFFFAOYSA-N
Formula: C11H14INO
SMILES: Cc1ccc(NC(=O)C(C)C)c(I)c1
Mol. weight [g/mol]: 303.14

Physical Properties

Property code	Value	Unit	Source
gf	151.04	kJ/mol	Joback Method
hf	-44.30	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.194		Crippen Method
mcvol	179.460	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	684.46	K	Joback Method
tc	928.36	K	Joback Method
tf	410.84	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.97	J/mol×K	684.46	Joback Method
cpg	432.01	J/mol×K	725.11	Joback Method
cpg	444.10	J/mol×K	765.76	Joback Method
cpg	455.28	J/mol×K	806.41	Joback Method
cpg	465.61	J/mol×K	847.06	Joback Method
cpg	475.15	J/mol×K	887.71	Joback Method
cpg	483.95	J/mol×K	928.36	Joback Method

Sources

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=U307326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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