2-Butenamide, N-(2-iodo-4-methylphenyl)-3-methyl-

Inchi: InChI=1S/C12H14INO/c1-8(2)6-12(15)14-11-5-4-9(3)7-10(11)13/h4-7H,1-3H3,(H,14,15)
InchiKey: BYSKACWESUBYER-UHFFFAOYSA-N
Formula: C12H14INO
SMILES: CC(C)=CC(=O)Nc1ccc(C)cc1I
Mol. weight [g/mol]: 315.15

Physical Properties

Property code	Value	Unit	Source
gf	233.57	kJ/mol	Joback Method
hf	47.77	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.504		Crippen Method
mcvol	189.250	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	711.82	K	Joback Method
tc	959.53	K	Joback Method
tf	418.07	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.99	J/mol×K	711.82	Joback Method
cpg	457.86	J/mol×K	753.11	Joback Method
cpg	469.79	J/mol×K	794.39	Joback Method
cpg	480.85	J/mol×K	835.68	Joback Method
cpg	491.15	J/mol×K	876.96	Joback Method
cpg	500.75	J/mol×K	918.25	Joback Method
cpg	509.74	J/mol×K	959.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307273&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