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

Inchi: InChI=1S/C12H16INO/c1-3-4-5-12(15)14-11-7-6-9(2)8-10(11)13/h6-8H,3-5H2,1-2H3,(H,1

InchiKey: JETUZJGSOPXQPU-UHFFFAOYSA-N

Formula: C12H16INO

SMILES: CCCCC(=O)Nc1ccc(C)cc1I

Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	161.90	kJ/mol	Joback Method
hf	-59.66	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.728		Crippen Method
mcvol	193.550	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	2096.00		NIST Webbook
tb	707.78	K	Joback Method
tc	941.98	K	Joback Method
tf	437.11	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.14	J/mol×K	707.78	Joback Method
cpg	482.49	J/mol×K	746.81	Joback Method
cpg	494.91	J/mol×K	785.85	Joback Method
cpg	506.45	J/mol×K	824.88	Joback Method
cpg	517.17	J/mol×K	863.92	Joback Method
cpg	527.13	J/mol×K	902.95	Joback Method
cpg	536.37	J/mol×K	941.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306897&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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