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

Inchi: InChI=1S/C13H18INO/c1-3-4-5-6-13(16)15-12-8-7-10(2)9-11(12)14/h7-9H,3-6H2,1-2H3,(
InchiKey: OELSFTUIARSGFV-UHFFFAOYSA-N
Formula: C13H18INO
SMILES: CCCCCC(=O)Nc1ccc(C)cc1I
Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	170.32	kJ/mol	Joback Method
hf	-80.30	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.118		Crippen Method
mcvol	207.640	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	2199.00		NIST Webbook
tb	730.66	K	Joback Method
tc	960.53	K	Joback Method
tf	448.38	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.18	J/mol×K	730.66	Joback Method
cpg	535.03	J/mol×K	768.97	Joback Method
cpg	547.94	J/mol×K	807.28	Joback Method
cpg	559.96	J/mol×K	845.59	Joback Method
cpg	571.14	J/mol×K	883.91	Joback Method
cpg	581.54	J/mol×K	922.22	Joback Method
cpg	591.22	J/mol×K	960.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307293&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