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

Inchi: InChI=1S/C15H22INO/c1-3-4-5-6-7-8-15(18)17-14-10-9-12(2)11-13(14)16/h9-11H,3-8H2
InchiKey: XEWHNRADDVXZAF-UHFFFAOYSA-N
Formula: C15H22INO
SMILES: CCCCCCCC(=O)Nc1ccc(C)cc1I
Mol. weight [g/mol]: 359.25

Physical Properties

Property code	Value	Unit	Source
gf	187.16	kJ/mol	Joback Method
hf	-121.58	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.899		Crippen Method
mcvol	235.820	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	776.42	K	Joback Method
tc	999.04	K	Joback Method
tf	470.92	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.87	J/mol×K	776.42	Joback Method
cpg	643.52	J/mol×K	813.52	Joback Method
cpg	657.20	J/mol×K	850.63	Joback Method
cpg	669.97	J/mol×K	887.73	Joback Method
cpg	681.90	J/mol×K	924.83	Joback Method
cpg	693.02	J/mol×K	961.94	Joback Method
cpg	703.41	J/mol×K	999.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306930&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