Propanamide, N-(2-iodo-4-methylphenyl)-3-phenyl-

Inchi: InChI=1S/C16H16INO/c1-12-7-9-15(14(17)11-12)18-16(19)10-8-13-5-3-2-4-6-13/h2-7,9,1

InchiKey: IMJDTVSOVXJMMY-UHFFFAOYSA-N

Formula: C16H16INO

SMILES: Cc1ccc(NC(=O)CCc2ccccc2)c(I)c1

Mol. weight [g/mol]: 365.21

Physical Properties

Property code	Value	Unit	Source
gf	307.99	kJ/mol	Joback Method
hf	94.31	kJ/mol	Joback Method
hfus	35.60	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.171		Crippen Method
mcvol	226.150	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	825.98	K	Joback Method
tc	1083.56	K	Joback Method
tf	508.61	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.36	J/mol×K	825.98	Joback Method
cpg	602.67	J/mol×K	868.91	Joback Method
cpg	614.85	J/mol×K	911.84	Joback Method
cpg	625.99	J/mol×K	954.77	Joback Method
cpg	636.21	J/mol×K	997.70	Joback Method
cpg	645.61	J/mol×K	1040.63	Joback Method
cpg	654.29	J/mol×K	1083.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308121&Units=SI

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