Acetamide, N-(2-iodo-4-methylphenyl)-2-acetoxy-

Inchi: InChI=1S/C11H12INO3/c1-7-3-4-10(9(12)5-7)13-11(15)6-16-8(2)14/h3-5H,6H2,1-2H3,(H

InchiKey: KOZRCZQJHRNZSB-UHFFFAOYSA-N

Formula: C11H12INO3

SMILES: CC(=O)OCC(=O)Nc1ccc(C)cc1I

Mol. weight [g/mol]: 333.12

Physical Properties

Property code	Value	Unit	Source
gf	-80.44	kJ/mol	Joback Method
hf	-283.82	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.101		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	761.19	K	Joback Method
tc	1001.85	K	Joback Method
tf	498.00	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.47	J/mol×K	761.19	Joback Method
cpg	463.38	J/mol×K	801.30	Joback Method
cpg	473.41	J/mol×K	841.41	Joback Method
cpg	482.56	J/mol×K	881.52	Joback Method
cpg	490.88	J/mol×K	921.63	Joback Method
cpg	498.39	J/mol×K	961.74	Joback Method
cpg	505.12	J/mol×K	1001.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307097&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