Propanamide, N-(2-iodo-4-methylphenyl)-2-bromo-

Inchi: InChI=1S/C10H11BrINO/c1-6-3-4-9(8(12)5-6)13-10(14)7(2)11/h3-5,7H,1-2H3,(H,13,14)
InchiKey: YEXPUYZNKNLKNE-UHFFFAOYSA-N
Formula: C10H11BrINO
SMILES: Cc1ccc(NC(=O)C(C)Br)c(I)c1
Mol. weight [g/mol]: 368.01

Physical Properties

Property code	Value	Unit	Source
gf	156.94	kJ/mol	Joback Method
hf	2.67	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.322		Crippen Method
mcvol	182.870	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	2042.00		NIST Webbook
tb	727.74	K	Joback Method
tc	987.66	K	Joback Method
tf	459.37	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.12	J/mol×K	727.74	Joback Method
cpg	410.96	J/mol×K	771.06	Joback Method
cpg	420.91	J/mol×K	814.38	Joback Method
cpg	430.05	J/mol×K	857.70	Joback Method
cpg	438.46	J/mol×K	901.02	Joback Method
cpg	446.20	J/mol×K	944.34	Joback Method
cpg	453.37	J/mol×K	987.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307479&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