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

Inchi: InChI=1S/C9H9BrINO/c1-6-2-3-8(7(11)4-6)12-9(13)5-10/h2-4H,5H2,1H3,(H,12,13)
InchiKey: PFOSUYUQTYUGIF-UHFFFAOYSA-N
Formula: C9H9BrINO
SMILES: Cc1ccc(NC(=O)CBr)c(I)c1
Mol. weight [g/mol]: 353.98

Physical Properties

Property code	Value	Unit	Source
gf	150.96	kJ/mol	Joback Method
hf	28.59	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.933		Crippen Method
mcvol	168.780	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	705.30	K	Joback Method
tc	965.99	K	Joback Method
tf	463.10	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.20	J/mol×K	705.30	Joback Method
cpg	360.03	J/mol×K	748.75	Joback Method
cpg	369.05	J/mol×K	792.20	Joback Method
cpg	377.32	J/mol×K	835.64	Joback Method
cpg	384.93	J/mol×K	879.09	Joback Method
cpg	391.94	J/mol×K	922.54	Joback Method
cpg	398.43	J/mol×K	965.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307423&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