Propanamide, N-(4-bromophenyl)-2,2-dimethyl-

Inchi: InChI=1S/C11H14BrNO/c1-11(2,3)10(14)13-9-6-4-8(12)5-7-9/h4-7H,1-3H3,(H,13,14)
InchiKey: ZXYSRVSPDUSHBX-UHFFFAOYSA-N
Formula: C11H14BrNO
SMILES: CC(C)(C)C(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 256.14
CAS: 24109-06-6

Physical Properties

Property code	Value	Unit	Source
gf	122.15	kJ/mol	Joback Method
hf	-86.84	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.434		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	649.71	K	Joback Method
tc	887.64	K	Joback Method
tf	417.48	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.31	J/mol×K	649.71	Joback Method
cpg	425.87	J/mol×K	689.37	Joback Method
cpg	438.36	J/mol×K	729.02	Joback Method
cpg	449.86	J/mol×K	768.68	Joback Method
cpg	460.46	J/mol×K	808.33	Joback Method
cpg	470.24	J/mol×K	847.99	Joback Method
cpg	479.29	J/mol×K	887.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24109066&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