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

Inchi: InChI=1S/C10H12BrNO/c1-7(2)10(13)12-9-5-3-8(11)4-6-9/h3-7H,1-2H3,(H,12,13)
InchiKey: AVQYIQZFJLEKGK-UHFFFAOYSA-N
Formula: C10H12BrNO
SMILES: CC(C)C(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 242.11

Physical Properties

Property code	Value	Unit	Source
gf	108.45	kJ/mol	Joback Method
hf	-62.73	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.044		Crippen Method
mcvol	157.050	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	629.62	K	Joback Method
tc	863.24	K	Joback Method
tf	388.79	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.75	J/mol×K	629.62	Joback Method
cpg	373.39	J/mol×K	668.56	Joback Method
cpg	385.12	J/mol×K	707.49	Joback Method
cpg	395.99	J/mol×K	746.43	Joback Method
cpg	406.04	J/mol×K	785.37	Joback Method
cpg	415.34	J/mol×K	824.30	Joback Method
cpg	423.92	J/mol×K	863.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307323&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