2-Butenamide, N-(4-bromophenyl)-3-methyl-

Inchi: InChI=1S/C11H12BrNO/c1-8(2)7-11(14)13-10-5-3-9(12)4-6-10/h3-7H,1-2H3,(H,13,14)
InchiKey: BJPQRVCCAISNSI-UHFFFAOYSA-N
Formula: C11H12BrNO
SMILES: CC(C)=CC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 254.12

Physical Properties

Property code	Value	Unit	Source
gf	190.98	kJ/mol	Joback Method
hf	29.34	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.354		Crippen Method
mcvol	166.840	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1953.00		NIST Webbook
tb	656.98	K	Joback Method
tc	894.89	K	Joback Method
tf	396.02	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.45	J/mol×K	656.98	Joback Method
cpg	398.97	J/mol×K	696.63	Joback Method
cpg	410.55	J/mol×K	736.28	Joback Method
cpg	421.27	J/mol×K	775.93	Joback Method
cpg	431.21	J/mol×K	815.58	Joback Method
cpg	440.44	J/mol×K	855.23	Joback Method
cpg	449.05	J/mol×K	894.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307271&Units=SI

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