Adamantane-1-carboxamide, N-(4-bromophenyl)-

Other names: 1-Adamantanecarboxamide, N-(4-bromophenyl)-
Inchi: InChI=1S/C17H20BrNO/c18-14-1-3-15(4-2-14)19-16(20)17-8-11-5-12(9-17)7-13(6-11)10
InchiKey: QBJMRSCAECWAKC-UHFFFAOYSA-N
Formula: C17H20BrNO
SMILES: O=C(Nc1ccc(Br)cc1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 334.25
CAS: 121768-29-4

Physical Properties

Property code	Value	Unit	Source
gf	326.78	kJ/mol	Joback Method
hf	5.21	kJ/mol	Joback Method
hfus	32.50	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.604		Crippen Method
mcvol	223.100	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	2668.00		NIST Webbook
tb	810.28	K	Joback Method
tc	1066.94	K	Joback Method
tf	552.64	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.81	J/mol×K	810.28	Joback Method
cpg	700.64	J/mol×K	853.06	Joback Method
cpg	719.11	J/mol×K	895.83	Joback Method
cpg	737.57	J/mol×K	938.61	Joback Method
cpg	756.38	J/mol×K	981.38	Joback Method
cpg	775.91	J/mol×K	1024.16	Joback Method
cpg	796.50	J/mol×K	1066.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121768294&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