Cyclopropanecarbonitrile, 1-(p-bromophenyl)-2-[p-(dimethylamino)phenyl]-

Inchi: InChI=1S/C18H17BrN2/c1-21(2)16-9-3-13(4-10-16)17-11-18(17,12-20)14-5-7-15(19)8-6-

InchiKey: ZORJIKKKWXKFTI-UHFFFAOYSA-N

Formula: C18H17BrN2

SMILES: CN(C)c1ccc(C2CC2(C#N)c2ccc(Br)cc2)cc1

Mol. weight [g/mol]: 341.25

CAS: 32589-49-4

Physical Properties

Property code	Value	Unit	Source
gf	612.07	kJ/mol	Joback Method
hf	361.71	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Joback Method
ie	7.10 ± 0.05	eV	NIST Webbook
log10ws	-5.20		Crippen Method
logp	4.464		Crippen Method
mcvol	234.960	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	857.55	K	Joback Method
tc	1119.45	K	Joback Method
tf	565.36	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.35	J/mol×K	857.55	Joback Method
cpg	684.02	J/mol×K	901.20	Joback Method
cpg	700.66	J/mol×K	944.85	Joback Method
cpg	717.59	J/mol×K	988.50	Joback Method
cpg	735.13	J/mol×K	1032.15	Joback Method
cpg	753.59	J/mol×K	1075.80	Joback Method
cpg	773.30	J/mol×K	1119.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32589494&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume