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

Inchi: InChI=1S/C19H20N2/c1-14-4-8-16(9-5-14)19(13-20)12-18(19)15-6-10-17(11-7-15)21(2)3

InchiKey: ISNPIBKQKCKDSJ-UHFFFAOYSA-N

Formula: C19H20N2

SMILES: Cc1ccc(C2(C#N)CC2c2ccc(N(C)C)cc2)cc1

Mol. weight [g/mol]: 276.38

CAS: 32589-51-8

Physical Properties

Property code	Value	Unit	Source
gf	606.17	kJ/mol	Joback Method
hf	314.74	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
ie	6.80 ± 0.07	eV	NIST Webbook
log10ws	-4.51		Crippen Method
logp	4.010		Crippen Method
mcvol	231.550	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
tb	814.27	K	Joback Method
tc	1062.45	K	Joback Method
tf	516.83	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.93	J/mol×K	814.27	Joback Method
cpg	704.67	J/mol×K	855.63	Joback Method
cpg	721.95	J/mol×K	897.00	Joback Method
cpg	739.02	J/mol×K	938.36	Joback Method
cpg	756.16	J/mol×K	979.73	Joback Method
cpg	773.62	J/mol×K	1021.09	Joback Method
cpg	791.66	J/mol×K	1062.45	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=C32589518&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
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