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

Inchi: InChI=1S/C18H18N2/c1-20(2)16-10-8-14(9-11-16)17-12-18(17,13-19)15-6-4-3-5-7-15/h3

InchiKey: YZTXKMCIZNWIQY-UHFFFAOYSA-N

Formula: C18H18N2

SMILES: CN(C)c1ccc(C2CC2(C#N)c2ccccc2)cc1

Mol. weight [g/mol]: 262.35

CAS: 6114-58-5

Physical Properties

Property code	Value	Unit	Source
gf	607.38	kJ/mol	Joback Method
hf	346.85	kJ/mol	Joback Method
hfus	27.50	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
ie	6.90 ± 0.10	eV	NIST Webbook
log10ws	-4.03		Crippen Method
logp	3.701		Crippen Method
mcvol	217.460	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
tb	786.41	K	Joback Method
tc	1038.95	K	Joback Method
tf	493.04	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.77	J/mol×K	786.41	Joback Method
cpg	649.00	J/mol×K	828.50	Joback Method
cpg	665.64	J/mol×K	870.59	Joback Method
cpg	681.98	J/mol×K	912.68	Joback Method
cpg	698.29	J/mol×K	954.77	Joback Method
cpg	714.86	J/mol×K	996.86	Joback Method
cpg	731.96	J/mol×K	1038.95	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=C6114585&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