2-Carbophenyl-5-cyano-6-phenyl-2,3-dihydro-1,4-

Inchi: InChI=1S/C19H15NO2/c20-13-16-11-12-17(18(21)14-7-3-1-4-8-14)22-19(16)15-9-5-2-6-
InchiKey: LIBZLYMICHBNOW-UHFFFAOYSA-N
Formula: C19H15NO2
SMILES: N#CC1=C(c2ccccc2)OC(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	287.21	kJ/mol	Joback Method
hf	47.03	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.983		Crippen Method
mcvol	224.710	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	899.05	K	Joback Method
tc	1165.87	K	Joback Method
tf	531.40	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.08	J/mol×K	899.05	Joback Method
cpg	680.94	J/mol×K	943.52	Joback Method
cpg	692.36	J/mol×K	987.99	Joback Method
cpg	702.48	J/mol×K	1032.46	Joback Method
cpg	711.38	J/mol×K	1076.93	Joback Method
cpg	719.19	J/mol×K	1121.40	Joback Method
cpg	726.01	J/mol×K	1165.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002760&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume