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

Inchi: InChI=1S/C18H17N3O2/c1-20(2)15-7-3-13(4-8-15)17-11-18(17,12-19)14-5-9-16(10-6-14
InchiKey: WQAFEGBITDYAKW-UHFFFAOYSA-N
Formula: C18H17N3O2
SMILES: CN(C)c1ccc(C2CC2(C#N)c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 307.35
CAS: 28752-34-3

Physical Properties

Property code	Value	Unit	Source
gf	633.30	kJ/mol	Joback Method
hf	324.62	kJ/mol	Joback Method
hfus	38.48	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Joback Method
ie	8.30 ± 0.07	eV	NIST Webbook
log10ws	-4.68		Crippen Method
logp	3.610		Crippen Method
mcvol	234.880	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
tb	943.23	K	Joback Method
tc	1211.10	K	Joback Method
tf	649.17	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.80	J/mol×K	943.23	Joback Method
cpg	754.45	J/mol×K	987.88	Joback Method
cpg	772.53	J/mol×K	1032.52	Joback Method
cpg	791.37	J/mol×K	1077.17	Joback Method
cpg	811.32	J/mol×K	1121.81	Joback Method
cpg	832.70	J/mol×K	1166.46	Joback Method
cpg	855.84	J/mol×K	1211.10	Joback Method

Sources

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=C28752343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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