Cyclopropanecarbonitrile, 1-(p-chlorophenyl)-2-(p-methoxyphenyl)-

Inchi: InChI=1S/C17H14ClNO/c1-20-15-8-2-12(3-9-15)16-10-17(16,11-19)13-4-6-14(18)7-5-13/

InchiKey: UKBFLNJUMCRCGX-UHFFFAOYSA-N

Formula: C17H14ClNO

SMILES: COc1ccc(C2CC2(C#N)c2ccc(Cl)cc2)cc1

Mol. weight [g/mol]: 283.75

CAS: 32589-54-1

Physical Properties

Property code	Value	Unit	Source
gf	361.62	kJ/mol	Joback Method
hf	140.53	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
ie	7.70 ± 0.05	eV	NIST Webbook
log10ws	-4.93		Crippen Method
logp	4.297		Crippen Method
mcvol	211.500	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	815.92	K	Joback Method
tc	1076.27	K	Joback Method
tf	513.97	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.97	J/mol×K	815.92	Joback Method
cpg	601.38	J/mol×K	859.31	Joback Method
cpg	616.43	J/mol×K	902.70	Joback Method
cpg	631.39	J/mol×K	946.10	Joback Method
cpg	646.51	J/mol×K	989.49	Joback Method
cpg	662.02	J/mol×K	1032.88	Joback Method
cpg	678.19	J/mol×K	1076.27	Joback Method

Sources

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=C32589541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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