1,1,2,2-Cyclobutanetetracarbonitrile, 3-methoxy-3-phenyl-

Inchi: InChI=1S/C15H10N4O/c1-20-15(12-5-3-2-4-6-12)7-13(8-16,9-17)14(15,10-18)11-19/h2-6

InchiKey: NFNVEVHERDVBKE-UHFFFAOYSA-N

Formula: C15H10N4O

SMILES: COC1(c2ccccc2)CC(C#N)(C#N)C1(C#N)C#N

Mol. weight [g/mol]: 262.27

CAS: 73408-16-9

Physical Properties

Property code	Value	Unit	Source
gf	632.31	kJ/mol	Joback Method
hf	482.58	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	91.60	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	1.999		Crippen Method
mcvol	198.980	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
tb	1002.41	K	Joback Method
tc	1275.21	K	Joback Method
tf	645.06	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.24	J/mol×K	1002.41	Joback Method
cpg	644.25	J/mol×K	1047.88	Joback Method
cpg	675.22	J/mol×K	1093.34	Joback Method
cpg	710.72	J/mol×K	1138.81	Joback Method
cpg	751.32	J/mol×K	1184.27	Joback Method
cpg	797.61	J/mol×K	1229.74	Joback Method
cpg	850.15	J/mol×K	1275.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73408169&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