Benzene, 1-methoxy-4-(2-cyano-2-phenylethenyl)

Other names: 4-Methoxy-«alpha»-phenylcinnamonitrile
Inchi: InChI=1S/C16H13NO/c1-18-16-9-7-13(8-10-16)11-15(12-17)14-5-3-2-4-6-14/h2-11H,1H3
InchiKey: VQADOVBGJXESGV-RVDMUPIBSA-N
Formula: C16H13NO
SMILES: COc1ccc(C=C(C#N)c2ccccc2)cc1
Mol. weight [g/mol]: 235.28
CAS: 5432-07-5

Physical Properties

Property code	Value	Unit	Source
chs	-8042.00	kJ/mol	NIST Webbook
chs	-8037.00	kJ/mol	NIST Webbook
gf	398.88	kJ/mol	Joback Method
hf	228.11	kJ/mol	Joback Method
hfs	-116.60	kJ/mol	NIST Webbook
hfs	-116.00	kJ/mol	NIST Webbook
hfus	26.47	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.759		Crippen Method
mcvol	191.730	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	752.36	K	Joback Method
tc	1004.70	K	Joback Method
tf	403.62	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.22	J/mol×K	752.36	Joback Method
cpg	516.07	J/mol×K	794.42	Joback Method
cpg	528.77	J/mol×K	836.47	Joback Method
cpg	540.40	J/mol×K	878.53	Joback Method

cpg	551.06	J/mol×K	920.59	Joback Method
cpg	560.82	J/mol×K	962.64	Joback Method
cpg	569.78	J/mol×K	1004.70	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=C5432075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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