3-Carbomethoxyamino-3-phenyl-2,3-dihydrobenzo

Inchi: InChI=1S/C16H15NO3/c1-19-15(18)17-16(12-7-3-2-4-8-12)11-20-14-10-6-5-9-13(14)16/h
InchiKey: CSHJGAJOYHKUIL-UHFFFAOYSA-N
Formula: C16H15NO3
SMILES: COC(=O)NC1(c2ccccc2)COc2ccccc21
Mol. weight [g/mol]: 269.30
CAS: 92963-36-5

Physical Properties

Property code	Value	Unit	Source
gf	123.64	kJ/mol	Joback Method
hf	-147.27	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.679		Crippen Method
mcvol	201.210	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	784.21	K	Joback Method
tc	1035.18	K	Joback Method
tf	528.67	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.66	J/mol×K	784.21	Joback Method
cpg	595.04	J/mol×K	826.04	Joback Method
cpg	609.86	J/mol×K	867.87	Joback Method
cpg	624.36	J/mol×K	909.69	Joback Method
cpg	638.78	J/mol×K	951.52	Joback Method
cpg	653.34	J/mol×K	993.35	Joback Method
cpg	668.30	J/mol×K	1035.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92963365&Units=SI

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