Morpholine-3-carboxylic acid, 2-phenyl, methyl ester, cis

Inchi: InChI=1S/C12H15NO3/c1-15-12(14)10-11(16-8-7-13-10)9-5-3-2-4-6-9/h2-6,10-11,13H,7-

InchiKey: HZWHDMCEMDPHNT-GHMZBOCLSA-N

Formula: C12H15NO3

SMILES: COC(=O)C1NCCOC1c1ccccc1

Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-359.49	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	0.889		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1756.00		NIST Webbook
tb	667.31	K	Joback Method
tc	911.54	K	Joback Method
tf	458.32	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.50	J/mol×K	667.31	Joback Method
cpg	481.31	J/mol×K	708.02	Joback Method
cpg	497.75	J/mol×K	748.72	Joback Method
cpg	512.85	J/mol×K	789.43	Joback Method
cpg	526.60	J/mol×K	830.13	Joback Method
cpg	539.04	J/mol×K	870.84	Joback Method
cpg	550.17	J/mol×K	911.54	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=R331805&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume