

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

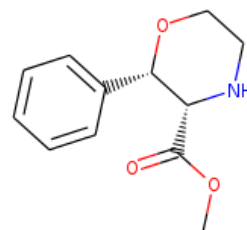
InChI: InChI=1S/C12H15NO3/c1-15-12(14)10-11(16-8-7-13-10)9-5-3-2-4-6-9/h2-6,10-11,13H,7-8H2,1H3/t10-,11-/m1/s1

InChI Key: HZWHDMCEMDPHNT-GHMZBOCLSA-N

Formula: C12H15NO3

SMILES: COC(=O)C1NCCOC1c1ccccc1

Molecular Weight: 221.25



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-53.02	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-359.49	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	34.14	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	65.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	0.89		Crippen Method
P_c	3069.34	kPa	Joback Method
T_{boil}	667.31	K	Joback Method
T_c	911.54	K	Joback Method
T_{fus}	458.32	K	Joback Method
V_c	0.61	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	463.50	J/mol×K	667.31	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/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,7-8H2,1H3/t10-,11-/m1/s1](http://webbook.nist.gov/cgi/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,7-8H2,1H3/t10-,11-/m1/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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