

Propanamide, n-(4-methoxyphenyl)-2-methyl-

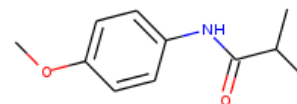
InChI: InChI=1S/C11H15NO2/c1-8(2)11(13)12-9-4-6-10(14-3)7-5-9/h4-8
H,1-3H3,(H,12,13)

InChI Key: VYJJVIXNXXKTFM-UHFFFAOYSA-N

Formula: C11H15NO2

SMILES: COc1ccc(NC(=O)C(C)C)cc1

Molecular Weight: 193.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-2.45	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-241.92	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.26	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	58.22	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.29		Crippen Method
P_c	2796.51	kPa	Joback Method
T_{boil}	608.76	K	Joback Method
T_c	823.24	K	Joback Method
T_{fus}	362.49	K	Joback Method
V_c	0.60	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	396.17	J/mol×K	608.76	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H15NO2/c1-8\(2\)11\(13\)12-9-4-6-10\(14-3\)7-5-9/h4-8H,1-3H3,\(H,12,13\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H15NO2/c1-8(2)11(13)12-9-4-6-10(14-3)7-5-9/h4-8H,1-3H3,(H,12,13))

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).

$\log P_{oct/wat}$: 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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