

2-((2-Ethoxyethoxy)carbonyl)benzoic acid

InChI: InChI=1S/C12H14O5/c1-2-16-7-8-17-12(15)10-6-4-3-5-9(10)11(13)14/h3-6H,2,7-8H2,1H3,(H,13,14)

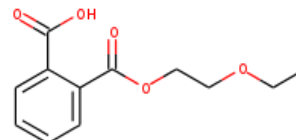
InChI Key: FCJKZKYOELZWNI-UHFFFAOYSA-N

Formula: C12H14O5

SMILES: CCOCOC(=O)c1ccccc1C(=O)O

Molecular Weight: 238.24

CAS: 735274-50-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-451.72	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-707.78	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.15	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.23	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.58		Crippen Method
P_c	2859.68	kPa	Joback Method
T_{boil}	750.38	K	Joback Method
T_c	950.99	K	Joback Method
T_{fus}	469.08	K	Joback Method
V_c	0.67	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	487.48	J/mol×K	750.38	Joback Method
η	0.00	Paxs	750.38	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O5/c1-2-16-7-8-17-12\(15\)10-6-4-3-5-9\(10\)11\(13\)14/h3-6H,2,7-8H2,1H3,\(H,13,14\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O5/c1-2-16-7-8-17-12(15)10-6-4-3-5-9(10)11(13)14/h3-6H,2,7-8H2,1H3,(H,13,14))

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

Legend

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

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: 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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