

Glutaric acid, but-3-yn-2-yl isopropyl ester

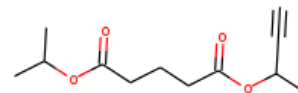
InChI: InChI=1S/C12H18O4/c1-5-10(4)16-12(14)8-6-7-11(13)15-9(2)3/h1,9-10H,6-8H2,2-4H3

InChI Key: GIMMHMKISOBPSW-UHFFFAOYSA-N

Formula: C₁₂H₁₈O₄

SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C)C

Molecular Weight: 226.27



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-199.49	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-499.27	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	28.34	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	59.70	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.67		Crippen Method
P_c	2237.64	kPa	Joback Method
T_{boil}	615.78	K	Joback Method
T_c	809.26	K	Joback Method
T_{fus}	386.29	K	Joback Method
V_c	0.71	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	473.55	J/mol×K	615.78	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O4/c1-5-10\(4\)16-12\(14\)8-6-7-11\(13\)15-9\(2\)3/h1,9-10H,6-8H2,2-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O4/c1-5-10(4)16-12(14)8-6-7-11(13)15-9(2)3/h1,9-10H,6-8H2,2-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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