

Glutaric acid, ethyl tridec-2-ynyl ester

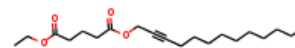
InChI: InChI=1S/C20H34O4/c1-3-5-6-7-8-9-10-11-12-13-14-18-24-20(22)17-15-16-19(21)23-4-2/h3-12,15-18H2,1-2H3

InChI Key: DBIPYAFNVFGNEN-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCCCCCCC#CCOC(=O)CCCC(=O)OCC

Molecular Weight: 338.48



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-147.52	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-673.43	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	56.25	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.58	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.80		Crippen Method
P_c	1200.62	kPa	Joback Method
T_{boil}	818.58	K	Joback Method
T_c	1009.33	K	Joback Method
T_{fus}	565.58	K	Joback Method
V_c	1.17	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	919.80	J/mol×K	818.58	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H34O4/c1-3-5-6-7-8-9-10-11-12-13-14-18-24-20\(22\)17-15-16-19\(21\)23-4-2/h3-12,15-18H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H34O4/c1-3-5-6-7-8-9-10-11-12-13-14-18-24-20(22)17-15-16-19(21)23-4-2/h3-12,15-18H2,1-2H3)

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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