

Glutaric acid, heptyl tridec-2-ynyl ester

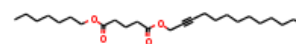
InChI: InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-14-16-18-23-29-25(27)21-19-20-24(26)28-22-17-15-8-6-4-2/h3-15,17,19-23H2,1-2H3

InChI Key: UNGGFRGILDTEBN-UHFFFAOYSA-N

Formula: C₂₅H₄₄O₄

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

Molecular Weight: 408.61



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-105.42	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-776.63	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	69.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	91.71	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.75		Crippen Method
P_c	882.62	kPa	Joback Method
T_{boil}	932.98	K	Joback Method
T_c	1142.70	K	Joback Method
T_{fus}	621.93	K	Joback Method
V_c	1.45	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1227.56	J/mol×K	932.98	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-14-16-18-23-29-25\(27\)21-19-20-24\(26\)28-22-17-15-8-6-4-2/h3-15,17,19-23H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-14-16-18-23-29-25(27)21-19-20-24(26)28-22-17-15-8-6-4-2/h3-15,17,19-23H2,1-2H3)

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).

$\log P_{oct/wat}$: 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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