

Adipic acid, dec-4-enyl pentyl ester

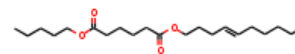
InChI: InChI=1S/C21H38O4/c1-3-5-7-8-9-10-11-15-19-25-21(23)17-13-12-16-20(22)24-18-14-6-4-2/h9-10H,3-8,11-19H2,1-2H3/b10-9+

InChI Key: GRJYQNCPDVDRDK-MDZDMXLPSA-N

Formula: C₂₁H₃₈O₄

SMILES: CCCCC=CCCCOC(=O)CCCCC(=O)OCCCCC

Molecular Weight: 354.52



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-261.68	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-849.15	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	55.92	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.61	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.74		Crippen Method
P_c	1047.33	kPa	Joback Method
T_{boil}	836.62	K	Joback Method
T_c	1025.83	K	Joback Method
T_{fus}	465.67	K	Joback Method
V_c	1.24	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1004.47	J/mol×K	836.62	Joback Method
η	0.00	Paxs	836.62	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H38O4/c1-3-5-7-8-9-10-11-15-19-25-21\(23\)17-13-12-16-20\(22\)24-18-14-6-4-2/h9-10H,3-8,11-19H2,1-2H3/b10-9+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H38O4/c1-3-5-7-8-9-10-11-15-19-25-21(23)17-13-12-16-20(22)24-18-14-6-4-2/h9-10H,3-8,11-19H2,1-2H3/b10-9+)

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

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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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