

Sebacic acid, 4-formylphenyl octyl ester

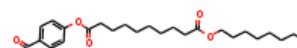
InChI: InChI=1S/C25H38O5/c1-2-3-4-5-10-13-20-29-24(27)14-11-8-6-7-9-12-15-25(28)30-23-18-16-22(21-26)17-19-23/h16-19,21H,2-15,20H2,1H3

InChI Key: WGXXYWJCDLDGFT-UHFFFAOYSA-N

Formula: C₂₅H₃₈O₅

SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1

Molecular Weight: 418.57



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-304.96	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-909.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	62.02	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	99.21	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.43		Crippen Method
P_c	1016.83	kPa	Joback Method
T_{boil}	1004.30	K	Joback Method
T_c	1230.41	K	Joback Method
T_{fus}	596.77	K	Joback Method
V_c	1.39	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1195.22	J/mol×K	1004.3	Joback Method
η	0.00	Paxs	1004.3	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H38O5/c1-2-3-4-5-10-13-20-29-24\(27\)14-11-8-6-7-9-12-15-25\(28\)30-23-18-16-22\(21-26\)17-19-23/h16-19,21H,2-15,20H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H38O5/c1-2-3-4-5-10-13-20-29-24(27)14-11-8-6-7-9-12-15-25(28)30-23-18-16-22(21-26)17-19-23/h16-19,21H,2-15,20H2,1H3)

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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