

Benzoic acid, 4-methoxy-, decyl ester

Other names: p-Methoxybenzoic acid, decyl ester.

InChI: InChI=1S/C18H28O3/c1-3-4-5-6-7-8-9-10-15-21-18(19)16-11-13-17(20-2)14-12-16/h11-14H,3-10,15H2,1-2H3

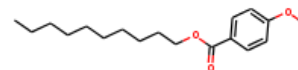
InChI Key: BENWKHCLHKJAMG-UHFFFAOYSA-N

Formula: C18H28O3

SMILES: CCCCCCCCCCOC(=O)c1ccc(OC)cc1

Molecular Weight: 292.41

CAS: 6974-04-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-135.46	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-566.81	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	40.00	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	70.17	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.993		Crippen Method
P_c	1478.15	kPa	Joback Method
T_{boil}	741.61	K	Joback Method
T_c	934.08	K	Joback Method
T_{fus}	425.95	K	Joback Method
V_c	0.978	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	740.43	J/mol×K	741.61	Joback Method
η	0.0000735	Paxs	741.61	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H28O3/c1-3-4-5-6-7-8-9-10-15-21-18\(19\)16-11-13-17\(20-2\)14-12-16/h11-14H,3-10,15H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H28O3/c1-3-4-5-6-7-8-9-10-15-21-18(19)16-11-13-17(20-2)14-12-16/h11-14H,3-10,15H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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