

Glutaric acid, 2-(2-methoxyethyl)heptyl pentyl ester

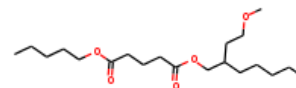
InChI: InChI=1S/C20H38O5/c1-4-6-8-11-18(14-16-23-3)17-25-20(22)13-10-12-19(21)24-15-9-7-5-2/h18H,4-17H2,1-3H3

InChI Key: XGPWORLFLGJDIV-UHFFFAOYSA-N

Formula: C20H38O5

SMILES: CCCCCOC(=O)CCCC(=O)OCC(CCCCC)CCOC

Molecular Weight: 358.51



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-457.76	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1083.23	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	50.79	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.45	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.67		Crippen Method
P_c	1071.46	kPa	Joback Method
T_{boil}	831.56	K	Joback Method
T_c	1019.41	K	Joback Method
T_{fus}	466.71	K	Joback Method
V_c	1.22	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1001.32	J/mol×K	831.56	Joback Method
η	0.00	Paxs	831.56	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H38O5/c1-4-6-8-11-18\(14-16-23-3\)17-25-20\(22\)13-10-12-19\(21\)24-15-9-7-5-2/h18H,4-17H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H38O5/c1-4-6-8-11-18(14-16-23-3)17-25-20(22)13-10-12-19(21)24-15-9-7-5-2/h18H,4-17H2,1-3H3)

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

Legend

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

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: 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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