# Fumaric acid, 8-chlorooctyl tridecyl ester

**Inchi:** InChI=1S/C25H45ClO4/c1-2-3-4-5-6-7-8-9-11-14-17-22-29-24(27)19-20-25(28)30-23-18-
**InchiKey:** KXJLNMQRVDAJCN-FMQUCBEESA-N
**Formula:** C25H45ClO4
**SMILES:** CCCCCCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCl
**Mol. weight [g/mol]:** 445.07

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -239.93 | kJ/mol | Joback Method |
| hf | -947.45 | kJ/mol | Joback Method |
| hfus | 70.48 | kJ/mol | Joback Method |
| hvap | 93.90 | kJ/mol | Joback Method |
| log10ws | -8.02 | | Crippen Method |
| logp | 7.519 | | Crippen Method |
| mcvol | 385.930 | ml/mol | McGowan Method |
| pc | 811.22 | kPa | Joback Method |
| rinpol | 3222.00 | | NIST Webbook |
| rinpol | 3222.00 | | NIST Webbook |
| tb | 965.57 | K | Joback Method |
| tc | 1186.60 | K | Joback Method |
| tf | 540.67 | K | Joback Method |
| vc | 1.512 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1283.75 | J/mol×K | 965.57 | Joback Method |
| cpg | 1303.05 | J/mol×K | 1002.41 | Joback Method |
| cpg | 1320.89 | J/mol×K | 1039.25 | Joback Method |
| cpg | 1337.34 | J/mol×K | 1076.09 | Joback Method |
| cpg | 1352.48 | J/mol×K | 1112.93 | Joback Method |
| cpg | 1366.35 | J/mol×K | 1149.76 | Joback Method |
| cpg | 1379.04 | J/mol×K | 1186.60 | Joback Method |
| dvisc | 0.0003323 | Pa×s | 540.67 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001554 | Pa×s | 611.49 | Joback Method |
| dvisc | 0.0000851 | Pa×s | 682.30 | Joback Method |
| dvisc | 0.0000522 | Pa×s | 753.12 | Joback Method |
| dvisc | 0.0000348 | Pa×s | 823.94 | Joback Method |
| dvisc | 0.0000247 | Pa×s | 894.75 | Joback Method |
| dvisc | 0.0000185 | Pa×s | 965.57 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348539&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |