# Fumaric acid, dodecyl 3-oxobut-2-yl ester

**Inchi:** InChI=1S/C20H34O5/c1-4-5-6-7-8-9-10-11-12-13-16-24-19(22)14-15-20(23)25-18(3)17(2
**InchiKey:** TYYXXOUHSFLVKB-CCEZHUSRSA-N
**Formula:** C20H34O5
**SMILES:** CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
**Mol. weight [g/mol]:** 354.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -401.46 | kJ/mol | Joback Method |
| hf | -946.37 | kJ/mol | Joback Method |
| hfus | 51.41 | kJ/mol | Joback Method |
| hvap | 84.74 | kJ/mol | Joback Method |
| log10ws | -5.17 | | Crippen Method |
| logp | 4.527 | | Crippen Method |
| mcvol | 304.810 | ml/mol | McGowan Method |
| pc | 1170.42 | kPa | Joback Method |
| rinpol | 2458.00 | | NIST Webbook |
| rinpol | 2458.00 | | NIST Webbook |
| tb | 867.17 | K | Joback Method |
| tc | 1064.01 | K | Joback Method |
| tf | 489.33 | K | Joback Method |
| vc | 1.183 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 965.67 | J/mol×K | 867.17 | Joback Method |
| cpg | 981.98 | J/mol×K | 899.98 | Joback Method |
| cpg | 997.21 | J/mol×K | 932.78 | Joback Method |
| cpg | 1011.39 | J/mol×K | 965.59 | Joback Method |
| cpg | 1024.54 | J/mol×K | 998.40 | Joback Method |
| cpg | 1036.70 | J/mol×K | 1031.21 | Joback Method |
| cpg | 1047.89 | J/mol×K | 1064.01 | Joback Method |
| dvisc | 0.0006917 | Pa×s | 489.33 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003289 | Pa×s | 552.30 | Joback Method |
| dvisc | 0.0001821 | Pa×s | 615.28 | Joback Method |
| dvisc | 0.0001125 | Pa×s | 678.25 | Joback Method |
| dvisc | 0.0000755 | Pa×s | 741.22 | Joback Method |
| dvisc | 0.0000539 | Pa×s | 804.20 | Joback Method |
| dvisc | 0.0000404 | Pa×s | 867.17 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=U348826&Units=SI |

# 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 |