# Succinic acid, hept-2-yl 1-bromo-3,3,3-trifluoroprop-2-yl ester

**Inchi:** InChI=1S/C14H22BrF3O4/c1-3-4-5-6-10(2)21-12(19)7-8-13(20)22-11(9-15)14(16,17)18/h

**InchiKey:** UUFMAXYQDGWBLV-UHFFFAOYSA-N

**Formula:** C14H22BrF3O4

**SMILES:** CCCCCC(C)OC(=O)CCC(=O)OC(CBr)C(F)(F)F

**Mol. weight [g/mol]:** 391.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -972.99 | kJ/mol | Joback Method |
| hf | -1403.20 | kJ/mol | Joback Method |
| hfus | 37.65 | kJ/mol | Joback Method |
| hvap | 66.98 | kJ/mol | Joback Method |
| log10ws | -4.73 | | Crippen Method |
| logp | 4.148 | | Crippen Method |
| mcvol | 245.810 | ml/mol | McGowan Method |
| pc | 1598.72 | kPa | Joback Method |
| rinpol | 1746.00 | | NIST Webbook |
| rinpol | 1746.00 | | NIST Webbook |
| tb | 732.16 | K | Joback Method |
| tc | 914.22 | K | Joback Method |
| tf | 425.85 | K | Joback Method |
| vc | 0.961 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 694.24 | J/mol×K | 732.16 | Joback Method |
| cpg | 707.94 | J/mol×K | 762.50 | Joback Method |
| cpg | 720.84 | J/mol×K | 792.85 | Joback Method |
| cpg | 732.96 | J/mol×K | 823.19 | Joback Method |
| cpg | 744.34 | J/mol×K | 853.54 | Joback Method |
| cpg | 754.98 | J/mol×K | 883.88 | Joback Method |
| cpg | 764.93 | J/mol×K | 914.22 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390825&Units=SI |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |