

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

<b>Inchi:</b>	InChI=1S/C20H30BrF3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-27-18(25)13-14-19(26)28-17(
<b>InchiKey:</b>	RQLHKFVRZOOXKV-UHFFFAOYSA-N
<b>Formula:</b>	C20H30BrF3O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCC(=O)OC(CBr)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	471.35

## Physical Properties

Property code	Value	Unit	Source
gf	-717.23	kJ/mol	Joback Method
hf	-1249.46	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.713		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	878.88	K	Joback Method
tc	1078.04	K	Joback Method
tf	614.57	K	Joback Method
vc	1.264	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.23	J/molxK	878.88	Joback Method
cpg	1002.28	J/molxK	912.07	Joback Method
cpg	1016.31	J/molxK	945.27	Joback Method
cpg	1029.37	J/molxK	978.46	Joback Method
cpg	1041.51	J/molxK	1011.66	Joback Method
cpg	1052.77	J/molxK	1044.85	Joback Method
cpg	1063.19	J/molxK	1078.04	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390836&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

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

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