

# Malonic acid, 2-butyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C11H20O4/c1-5-9(4)15-11(13)6-10(12)14-7-8(2)3/h8-9H,5-7H2,1-4H3
<b>InchiKey:</b>	LNZJNFXUORACEO-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O4
<b>SMILES:</b>	CCC(C)OC(=O)CC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	216.27

## Physical Properties

Property code	Value	Unit	Source
gf	-430.98	kJ/mol	Joback Method
hf	-770.53	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.917		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpola	1298.00		NIST Webbook
rinpola	1298.00		NIST Webbook
tb	602.78	K	Joback Method
tc	787.66	K	Joback Method
tf	328.05	K	Joback Method
vc	0.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.83	J/molxK	602.78	Joback Method
cpg	480.33	J/molxK	633.59	Joback Method
cpg	494.18	J/molxK	664.41	Joback Method
cpg	507.38	J/molxK	695.22	Joback Method
cpg	519.94	J/molxK	726.03	Joback Method
cpg	531.86	J/molxK	756.85	Joback Method
cpg	543.12	J/molxK	787.66	Joback Method
dvisc	0.0029767	Paxs	328.05	Joback Method

dvisc	0.0013297	Paxs	373.84	Joback Method
dvisc	0.0007082	Paxs	419.63	Joback Method
dvisc	0.0004269	Paxs	465.41	Joback Method
dvisc	0.0002818	Paxs	511.20	Joback Method
dvisc	0.0001992	Paxs	556.99	Joback Method
dvisc	0.0001484	Paxs	602.78	Joback Method

## Sources

<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=U349068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349068&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hvap:</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>mcvol:</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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