

# Glutaric acid, but-3-en-2-yl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C20H22O4/c1-3-15(2)24-20(22)10-6-9-19(21)23-14-16-11-12-17-7-4-5-8-18(17)
InchiKey:	QKJLXLVZCAPFR-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	326.39

## Physical Properties

Property code	Value	Unit	Source
gf	-55.49	kJ/mol	Joback Method
hf	-409.45	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	81.95	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.171		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	856.46	K	Joback Method
tc	1075.20	K	Joback Method
tf	514.36	K	Joback Method
vc	0.993	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.98	J/molxK	856.46	Joback Method
cpg	790.17	J/molxK	892.92	Joback Method
cpg	803.28	J/molxK	929.37	Joback Method
cpg	815.39	J/molxK	965.83	Joback Method
cpg	826.54	J/molxK	1002.29	Joback Method
cpg	836.79	J/molxK	1038.75	Joback Method
cpg	846.20	J/molxK	1075.20	Joback Method
dvisc	0.0007908	Paxs	514.36	Joback Method

dvisc	0.0004787	Paxs	571.38	Joback Method
dvisc	0.0003174	Paxs	628.39	Joback Method
dvisc	0.0002254	Paxs	685.41	Joback Method
dvisc	0.0001686	Paxs	742.43	Joback Method
dvisc	0.0001315	Paxs	799.44	Joback Method
dvisc	0.0001060	Paxs	856.46	Joback Method

## Sources

<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>
<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=U405249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405249&amp;Units=SI</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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