

# Butyric acid, 2-naphthyl ester

<b>Inchi:</b>	InChI=1S/C14H14O2/c1-2-5-14(15)16-13-9-8-11-6-3-4-7-12(11)10-13/h3-4,6-10H,2,5H2
<b>InchiKey:</b>	KCWQXDQUK LJUEU-UHFFFAOYSA-N
<b>Formula:</b>	C14H14O2
<b>SMILES:</b>	CCCC(=O)Oc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	214.26

## Physical Properties

Property code	Value	Unit	Source
gf	42.51	kJ/mol	Joback Method
hf	-160.96	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.545		Crippen Method
mvol	172.340	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1768.00		NIST Webbook
tb	646.65	K	Joback Method
tc	872.78	K	Joback Method
tf	391.34	K	Joback Method
vc	0.657	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.01	J/molxK	646.65	Joback Method
cpg	448.60	J/molxK	684.34	Joback Method
cpg	462.19	J/molxK	722.03	Joback Method
cpg	474.83	J/molxK	759.72	Joback Method
cpg	486.57	J/molxK	797.41	Joback Method
cpg	497.48	J/molxK	835.09	Joback Method
cpg	507.61	J/molxK	872.78	Joback Method
dvisc	0.0014034	Paxs	391.34	Joback Method
dvisc	0.0009208	Paxs	433.89	Joback Method

dvisc	0.0006514	Paxs	476.44	Joback Method
dvisc	0.0004877	Paxs	519.00	Joback Method
dvisc	0.0003815	Paxs	561.55	Joback Method
dvisc	0.0003090	Paxs	604.10	Joback Method
dvisc	0.0002573	Paxs	646.65	Joback Method

## Sources

<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=U307519&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307519&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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