

# Butanoic acid, docosyl ester

<b>Other names:</b>	Docosanyl butyrate
<b>Inchi:</b>	InChI=1S/C26H52O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-28
<b>InchiKey:</b>	VCZVPMCCBMEIIG-UHFFFAOYSA-N
<b>Formula:</b>	C26H52O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CCC
<b>Mol. weight [g/mol]:</b>	396.69
<b>CAS:</b>	55373-87-0

## Physical Properties

Property code	Value	Unit	Source
gf	-65.88	kJ/mol	Joback Method
hf	-824.77	kJ/mol	Joback Method
hfus	65.88	kJ/mol	Joback Method
hvap	82.63	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	9.152		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpol	2781.00		NIST Webbook
rinpol	2781.00		NIST Webbook
tb	870.57	K	Joback Method
tc	1067.44	K	Joback Method
tf	454.94	K	Joback Method
vc	1.516	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.37	J/molxK	870.57	Joback Method
cpg	1308.31	J/molxK	903.38	Joback Method
cpg	1329.90	J/molxK	936.19	Joback Method
cpg	1350.19	J/molxK	969.01	Joback Method
cpg	1369.24	J/molxK	1001.82	Joback Method
cpg	1387.08	J/molxK	1034.63	Joback Method

cpg	1403.78	J/mol×K	1067.44	Joback Method
dvisc	0.0008279	Paxs	454.94	Joback Method
dvisc	0.0003338	Paxs	524.21	Joback Method
dvisc	0.0001664	Paxs	593.48	Joback Method
dvisc	0.0000959	Paxs	662.75	Joback Method
dvisc	0.0000614	Paxs	732.03	Joback Method
dvisc	0.0000424	Paxs	801.30	Joback Method
dvisc	0.0000311	Paxs	870.57	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373870&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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