

# Methyl cerebronate

<b>Inchi:</b>	InChI=1S/C25H50O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(2)
<b>InchiKey:</b>	MSVLAXSCPVNLFM-UHFFFAOYSA-N
<b>Formula:</b>	C25H50O3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCC(O)C(=O)OC
<b>Mol. weight [g/mol]:</b>	398.66
<b>CAS:</b>	2433-95-6

## Physical Properties

Property code	Value	Unit	Source
gf	-213.56	kJ/mol	Joback Method
hf	-961.64	kJ/mol	Joback Method
hfus	63.86	kJ/mol	Joback Method
hvap	96.69	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.732		Crippen Method
mvol	376.420	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	2868.30		NIST Webbook
rinpol	2868.30		NIST Webbook
tb	939.43	K	Joback Method
tc	1161.11	K	Joback Method
tf	489.49	K	Joback Method
vc	1.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.91	J/molxK	939.43	Joback Method
cpg	1322.71	J/molxK	976.38	Joback Method
cpg	1342.96	J/molxK	1013.32	Joback Method
cpg	1361.76	J/molxK	1050.27	Joback Method
cpg	1379.17	J/molxK	1087.22	Joback Method
cpg	1395.25	J/molxK	1124.16	Joback Method
cpg	1410.08	J/molxK	1161.11	Joback Method

dvisc	0.0004756	Paxs	489.49	Joback Method
dvisc	0.0001296	Paxs	564.48	Joback Method
dvisc	0.0000479	Paxs	639.47	Joback Method
dvisc	0.0000218	Paxs	714.46	Joback Method
dvisc	0.0000115	Paxs	789.45	Joback Method
dvisc	0.0000068	Paxs	864.44	Joback Method
dvisc	0.0000044	Paxs	939.43	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2433956&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2433956&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>
<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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