

# parethoxycaine

<b>Inchi:</b>	InChI=1S/C15H23NO3/c1-4-16(5-2)11-12-19-15(17)13-7-9-14(10-8-13)18-6-3/h7-10H,4-
<b>InchiKey:</b>	OWVVHQYOYSPNNE-UHFFFAOYSA-N
<b>Formula:</b>	C15H23NO3
<b>SMILES:</b>	CCOc1ccc(C(=O)OCCN(CC)CC)cc1
<b>Mol. weight [g/mol]:</b>	265.35

## Physical Properties

Property code	Value	Unit	Source
gf	-49.94	kJ/mol	Joback Method
hf	-437.36	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-2.71		Aqueous Solubility Prediction Method
logp	2.584		Crippen Method
mcvol	221.740	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
tb	685.41	K	Joback Method
tc	880.46	K	Joback Method
tf	424.61	K	Joback Method
vc	0.828	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.66	J/mol×K	685.41	Joback Method
cpg	630.12	J/mol×K	717.92	Joback Method
cpg	645.65	J/mol×K	750.43	Joback Method
cpg	660.26	J/mol×K	782.93	Joback Method
cpg	673.97	J/mol×K	815.44	Joback Method
cpg	686.80	J/mol×K	847.95	Joback Method
cpg	698.77	J/mol×K	880.46	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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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>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>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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