

# Pimelic acid, 4-bromo-2-methoxybenzyl octyl ester

Inchi:	InChI=1S/C23H35BrO5/c1-3-4-5-6-7-11-16-28-22(25)12-9-8-10-13-23(26)29-18-19-14-1
InchiKey:	ZSHRAIGIATXHBT-UHFFFAOYSA-N
Formula:	C23H35BrO5
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCc1ccc(Br)cc1OC
Mol. weight [g/mol]:	471.43

## Physical Properties

Property code	Value	Unit	Source
gf	-322.59	kJ/mol	Joback Method
hf	-899.95	kJ/mol	Joback Method
hfus	60.64	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.355		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	1003.44	K	Joback Method
tc	1228.50	K	Joback Method
tf	626.78	K	Joback Method
vc	1.343	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.30	J/molxK	1003.44	Joback Method
cpg	1139.46	J/molxK	1040.95	Joback Method
cpg	1152.08	J/molxK	1078.46	Joback Method
cpg	1163.20	J/molxK	1115.97	Joback Method
cpg	1172.84	J/molxK	1153.48	Joback Method
cpg	1181.03	J/molxK	1190.99	Joback Method
cpg	1187.81	J/molxK	1228.50	Joback Method
dvisc	0.0001712	Paxs	626.78	Joback Method

dvisc	0.0001022	Paxs	689.56	Joback Method
dvisc	0.0000665	Paxs	752.33	Joback Method
dvisc	0.0000463	Paxs	815.11	Joback Method
dvisc	0.0000339	Paxs	877.89	Joback Method
dvisc	0.0000259	Paxs	940.66	Joback Method
dvisc	0.0000204	Paxs	1003.44	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=U406589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406589&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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