

Benzoic acid, (-)-menthyl ester

Other names:	(-)-menthyl benzoate Benzoic acid, (-)-menthyl ester Menthyl benzoate
Inchi:	InChI=1S/C17H24O2/c1-12(2)15-10-9-13(3)11-16(15)19-17(18)14-7-5-4-6-8-14/h4-8,12-
InchiKey:	TTYVYRHNIVBWCB-UHFFFAOYSA-N
Formula:	C17H24O2
SMILES:	CC1CCC(C(C)C)C(OC(=O)c2ccccc2)C1
Mol. weight [g/mol]:	260.38

Physical Properties

Property code	Value	Unit	Source
hfus	27.07	kJ/mol	Joback Method
logp	4.304		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
tb	597.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.85	J/mol×K	889.93	Joback Method
cpg	761.01	J/mol×K	927.69	Joback Method
cpg	675.79	J/mol×K	738.87	Joback Method
cpg	695.79	J/mol×K	776.63	Joback Method
cpg	714.28	J/mol×K	814.40	Joback Method
cpg	731.29	J/mol×K	852.16	Joback Method
cpg	654.24	J/mol×K	701.10	Joback Method
dvisc	0.0005942	Pa×s	476.25	Joback Method
dvisc	0.0010363	Pa×s	420.04	Joback Method
dvisc	0.0021464	Pa×s	363.83	Joback Method
dvisc	0.0003831	Pa×s	532.46	Joback Method
dvisc	0.0002686	Pa×s	588.68	Joback Method
dvisc	0.0002004	Pa×s	644.89	Joback Method
dvisc	0.0001567	Pa×s	701.10	Joback Method
hvapt	69.90	kJ/mol	485.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6284351&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/90-415-1/Benzoic-acid-menthyl-ester.pdf>

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