

Cyclohexanol, 5-methyl-2-(1-methylethyl)-, benzoate, [1R-(1«alpha»,2«beta»,5«alpha»)]-

Other names: Benzoic acid, (-)-menthyl ester

(-)-menthyl benzoate

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]: 260.37

CAS: 6284-35-1

Physical Properties

Property code	Value	Unit	Source
gf	-22.66	kJ/mol	Joback Method
hf	-394.12	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.304		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
tb	701.10	K	Joback Method
tc	927.69	K	Joback Method
tf	363.83	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.01	J/molxK	927.69	Joback Method
cpg	654.24	J/molxK	701.10	Joback Method
cpg	675.79	J/molxK	738.87	Joback Method
cpg	695.79	J/molxK	776.63	Joback Method
cpg	714.28	J/molxK	814.40	Joback Method
cpg	731.29	J/molxK	852.16	Joback Method

cpg	746.85	J/molxK	889.93	Joback Method
dvisc	0.0001567	Paxs	701.10	Joback Method
dvisc	0.0021464	Paxs	363.83	Joback Method
dvisc	0.0010363	Paxs	420.04	Joback Method
dvisc	0.0005942	Paxs	476.25	Joback Method
dvisc	0.0003831	Paxs	532.47	Joback Method
dvisc	0.0002686	Paxs	588.68	Joback Method
dvisc	0.0002004	Paxs	644.89	Joback Method
hvapt	69.90	kJ/mol	485.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6284351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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