

Cyclohexanecarboxylic acid, 4-methoxy-, nonyl ester

Inchi:	InChI=1S/C17H32O3/c1-3-4-5-6-7-8-9-14-20-17(18)15-10-12-16(19-2)13-11-15/h15-16H
InchiKey:	CHGZPZFSWLCDBB-UHFFFAOYSA-N
Formula:	C17H32O3
SMILES:	CCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	284.43

Physical Properties

Property code	Value	Unit	Source
gf	-229.92	kJ/mol	Joback Method
hf	-737.25	kJ/mol	Joback Method
hfus	36.67	kJ/mol	Joback Method
hvap	65.12	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.485		Crippen Method
mvol	252.840	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	701.95	K	Joback Method
tc	889.80	K	Joback Method
tf	378.88	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.86	J/mol×K	701.95	Joback Method
cpg	782.49	J/mol×K	733.26	Joback Method
cpg	802.00	J/mol×K	764.57	Joback Method
cpg	820.42	J/mol×K	795.88	Joback Method
cpg	837.74	J/mol×K	827.18	Joback Method
cpg	853.97	J/mol×K	858.49	Joback Method
cpg	869.14	J/mol×K	889.80	Joback Method
dvisc	0.0016939	Paxs	378.88	Joback Method

dvisc	0.0008016	Paxs	432.72	Joback Method
dvisc	0.0004476	Paxs	486.57	Joback Method
dvisc	0.0002808	Paxs	540.41	Joback Method
dvisc	0.0001916	Paxs	594.26	Joback Method
dvisc	0.0001394	Paxs	648.11	Joback Method
dvisc	0.0001064	Paxs	701.95	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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