

Cyclohexanecarboxylic acid, 4-methoxy-, propyl ester

Inchi:	InChI=1S/C11H20O3/c1-3-8-14-11(12)9-4-6-10(13-2)7-5-9/h9-10H,3-8H2,1-2H3
InchiKey:	UTFGJWBPBDQEDK-UHFFFAOYSA-N
Formula:	C11H20O3
SMILES:	CCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	200.27

Physical Properties

Property code	Value	Unit	Source
gf	-280.44	kJ/mol	Joback Method
hf	-613.41	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	51.77	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.145		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1450.00		NIST Webbook
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tb	564.67	K	Joback Method
tc	765.00	K	Joback Method
tf	311.26	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.84	J/molxK	564.67	Joback Method
cpg	451.35	J/molxK	598.06	Joback Method
cpg	468.98	J/molxK	631.45	Joback Method
cpg	485.74	J/molxK	664.84	Joback Method
cpg	501.62	J/molxK	698.23	Joback Method
cpg	516.62	J/molxK	731.62	Joback Method
cpg	530.72	J/molxK	765.00	Joback Method
dvisc	0.0023664	Paxs	311.26	Joback Method

dvisc	0.0012260	Paxs	353.50	Joback Method
dvisc	0.0007309	Paxs	395.73	Joback Method
dvisc	0.0004815	Paxs	437.96	Joback Method
dvisc	0.0003413	Paxs	480.20	Joback Method
dvisc	0.0002558	Paxs	522.43	Joback Method
dvisc	0.0002002	Paxs	564.67	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U406190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
log10ws:	Log10 of Water solubility in mol/l
logp:	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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