

Cyclohexanecarboxylic acid, 4-methoxy-, pentadecyl ester

Inchi:	InChI=1S/C23H44O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-26-23(24)21-16-18-22(25-26)
InchiKey:	OUQFWRFMFWNXKB-UHFFFAOYSA-N
Formula:	C23H44O3
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	368.59

Physical Properties

Property code	Value	Unit	Source
gf	-179.40	kJ/mol	Joback Method
hf	-861.09	kJ/mol	Joback Method
hfus	52.21	kJ/mol	Joback Method
hvap	78.48	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.826		Crippen Method
mvol	337.380	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook
tb	839.23	K	Joback Method
tc	1031.09	K	Joback Method
tf	446.50	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.34	J/molxK	839.23	Joback Method
cpg	1150.87	J/molxK	871.21	Joback Method
cpg	1171.00	J/molxK	903.18	Joback Method
cpg	1189.76	J/molxK	935.16	Joback Method
cpg	1207.17	J/molxK	967.14	Joback Method
cpg	1223.25	J/molxK	999.12	Joback Method
cpg	1238.03	J/molxK	1031.09	Joback Method
dvisc	0.0009483	Paxs	446.50	Joback Method

dvisc	0.0004201	Paxs	511.95	Joback Method
dvisc	0.0002239	Paxs	577.41	Joback Method
dvisc	0.0001356	Paxs	642.87	Joback Method
dvisc	0.0000901	Paxs	708.32	Joback Method
dvisc	0.0000642	Paxs	773.77	Joback Method
dvisc	0.0000482	Paxs	839.23	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=U406203&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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