

Cyclohexanecarboxylic acid, 4-methoxy-, undecyl ester

Inchi:	InChI=1S/C19H36O3/c1-3-4-5-6-7-8-9-10-11-16-22-19(20)17-12-14-18(21-2)15-13-17/h
InchiKey:	SYLVEEBBBQYINJ-UHFFFAOYSA-N
Formula:	C19H36O3
SMILES:	CCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	312.49

Physical Properties

Property code	Value	Unit	Source
gf	-213.08	kJ/mol	Joback Method
hf	-778.53	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	69.57	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.266		Crippen Method
mvol	281.020	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2258.00		NIST Webbook
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tb	747.71	K	Joback Method
tc	934.53	K	Joback Method
tf	401.42	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.00	J/molxK	747.71	Joback Method
cpg	973.97	J/molxK	903.40	Joback Method
cpg	957.70	J/molxK	872.26	Joback Method
cpg	940.28	J/molxK	841.12	Joback Method
cpg	921.70	J/molxK	809.98	Joback Method
cpg	901.95	J/molxK	778.85	Joback Method
cpg	989.11	J/molxK	934.53	Joback Method
dvisc	0.0000828	Paxs	747.71	Joback Method

dvisc	0.0001091	Paxs	689.99	Joback Method
dvisc	0.0001513	Paxs	632.28	Joback Method
dvisc	0.0002238	Paxs	574.56	Joback Method
dvisc	0.0003615	Paxs	516.85	Joback Method
dvisc	0.0006585	Paxs	459.13	Joback Method
dvisc	0.0014256	Paxs	401.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406199&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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