

Cyclohexanecarboxylic acid, 4-methoxy-, octadecyl ester

Inchi:	InChI=1S/C26H50O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-29-26(27)24-19-2
InchiKey:	QQDXETMFWIDADB-UHFFFAOYSA-N
Formula:	C26H50O3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	410.67

Physical Properties

Property code	Value	Unit	Source
gf	-154.14	kJ/mol	Joback Method
hf	-923.01	kJ/mol	Joback Method
hfus	59.98	kJ/mol	Joback Method
hvap	85.16	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.996		Crippen Method
mcvol	379.650	ml/mol	McGowan Method
pc	810.30	kPa	Joback Method
rinsol	2980.00		NIST Webbook
tb	907.87	K	Joback Method
tc	1111.50	K	Joback Method
tf	480.31	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1322.05	J/molxK	907.87	Joback Method
cpg	1344.24	J/molxK	941.81	Joback Method
cpg	1364.77	J/molxK	975.75	Joback Method
cpg	1383.68	J/molxK	1009.68	Joback Method
cpg	1401.00	J/molxK	1043.62	Joback Method
cpg	1416.78	J/molxK	1077.56	Joback Method
cpg	1431.04	J/molxK	1111.50	Joback Method
dvisc	0.0006689	Paxs	480.31	Joback Method
dvisc	0.0002886	Paxs	551.57	Joback Method

dvisc	0.0001509	Paxs	622.83	Joback Method
dvisc	0.0000901	Paxs	694.09	Joback Method
dvisc	0.0000593	Paxs	765.35	Joback Method
dvisc	0.0000419	Paxs	836.61	Joback Method
dvisc	0.0000312	Paxs	907.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406206&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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