Cyclohexanecarboxylic acid, 4-methoxy-, heptadecyl ester

Inchi: InChI=1S/C25H48O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-28-25(26)23-18-20-2

InchiKey: MWWYWFZKLSEQQG-UHFFFAOYSA-N

Formula: C25H48O3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 396.65

Physical Properties

Property code	Value	Unit	Source
gf	-162.56	kJ/mol	Joback Method
hf	-902.37	kJ/mol	Joback Method
hfus	57.39	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.606		Crippen Method
mcvol	365.560	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	884.99	K	Joback Method
tc	1083.81	K	Joback Method
tf	469.04	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.33	J/mol×K	884.99	Joback Method
cpg	1279.27	J/mol×K	918.13	Joback Method
cpg	1299.65	J/mol×K	951.26	Joback Method
cpg	1318.50	J/mol×K	984.40	Joback Method
cpg	1335.86	J/mol×K	1017.54	Joback Method
cpg	1351.75	J/mol×K	1050.67	Joback Method
cpg	1366.21	J/mol×K	1083.81	Joback Method
dvisc	0.0007541	Pa×s	469.04	Joback Method

dvisc	0.0003281	Pa×s	538.37	Joback Method
dvisc	0.0001726	Pa×s	607.69	Joback Method
dvisc	0.0001036	Pa×s	677.01	Joback Method
dvisc	0.0000683	Pa×s	746.34	Joback Method
dvisc	0.0000484	Pa×s	815.66	Joback Method
dvisc	0.0000362	Pa×s	884.99	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=U406205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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