Cyclohexanecarboxylic acid, 4-methoxy-, tetradecyl ester

Inchi: InChI=1S/C22H42O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-25-22(23)20-15-17-21(24-2)18

InchiKey: REXRAODEVPBROT-UHFFFAOYSA-N

Formula: C22H42O3

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

Mol. weight [g/mol]: 354.57

Physical Properties

Property code	Value	Unit	Source
gf	-187.82	kJ/mol	Joback Method
hf	-840.45	kJ/mol	Joback Method
hfus	49.62	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.436		Crippen Method
mcvol	323.290	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	816.35	K	Joback Method
tc	1005.93	K	Joback Method
tf	435.23	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.19	J/mol×K	816.35	Joback Method
cpg	1087.56	J/mol×K	847.95	Joback Method
cpg	1107.59	J/mol×K	879.54	Joback Method
cpg	1126.31	J/mol×K	911.14	Joback Method
cpg	1143.73	J/mol×K	942.74	Joback Method
cpg	1159.89	J/mol×K	974.34	Joback Method
cpg	1174.79	J/mol×K	1005.93	Joback Method
dvisc	0.0010572	Pa×s	435.23	Joback Method

dvisc	0.0004730	Pa×s	498.75	Joback Method
dvisc	0.0002538	Pa×s	562.27	Joback Method
dvisc	0.0001545	Pa×s	625.79	Joback Method
dvisc	0.0001031	Pa×s	689.31	Joback Method
dvisc	0.0000736	Pa×s	752.83	Joback Method
dvisc	0.0000554	Pa×s	816.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406202&Units=SI

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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