1,2-Cyclohexanedicarboxylic acid, 5-methoxy-3-methylpentyl pentadecyl ester

Inchi: InChI=1S/C30H56O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-23-34-29(31)27-19-16-17-20

InchiKey: RHGLNHKVMWYFDL-UHFFFAOYSA-N

Formula: C30H56O5

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 496.76

Physical Properties

Property code	Value	Unit	Source
gf	-356.82	kJ/mol	Joback Method
hf	-1255.65	kJ/mol	Joback Method
hfus	69.60	kJ/mol	Joback Method
hvap	102.83	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	8.033		Crippen Method
mcvol	443.450	ml/mol	McGowan Method
pc	677.11	kPa	Joback Method
rinpol	3393.00		NIST Webbook
rinpol	3393.00		NIST Webbook
tb	1075.24	K	Joback Method
tc	1335.18	K	Joback Method
tf	582.55	K	Joback Method
vc	1.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1634.05	J/mol×K	1075.24	Joback Method
cpg	1703.22	J/mol×K	1291.86	Joback Method
cpg	1694.98	J/mol×K	1248.53	Joback Method
cpg	1684.01	J/mol×K	1205.21	Joback Method
cpg	1670.25	J/mol×K	1161.89	Joback Method
cpg	1653.62	J/mol×K	1118.56	Joback Method
cpg	1708.81	J/mol×K	1335.18	Joback Method
dvisc	0.0000106	Pa×s	1075.24	Joback Method

dvisc	0.0000143	Pa×s	993.12	Joback Method
dvisc	0.0000203	Pa×s	911.01	Joback Method
dvisc	0.0000311	Pa×s	828.89	Joback Method
dvisc	0.0000522	Pa×s	746.78	Joback Method
dvisc	0.0000997	Pa×s	664.66	Joback Method
dvisc	0.0002283	Pa×s	582.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339926&Units=SI
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

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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