cis-Cyclohex-4-en-1,2-dicarboxylic acid, pentadecyl phenethyl ester

Inchi: InChI=1S/C31H48O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-25-34-30(32)28-22-17-18-23-29
InchiKey: IOBZLESSXUAKOB-UHFFFAOYSA-N
Formula: C31H48O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]: 484.71

Physical Properties

Property code	Value	Unit	Source
gf	-98.59	kJ/mol	Joback Method
hf	-844.48	kJ/mol	Joback Method
hfus	69.79	kJ/mol	Joback Method
hvap	105.60	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.989		Crippen Method
mcvol	423.610	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3534.00		NIST Webbook
rinpol	3534.00		NIST Webbook
tb	1101.98	K	Joback Method
tc	1355.05	K	Joback Method
tf	613.77	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.02	J/mol×K	1101.98	Joback Method
cpg	1541.41	J/mol×K	1144.16	Joback Method
cpg	1555.61	J/mol×K	1186.34	Joback Method
cpg	1567.71	J/mol×K	1228.51	Joback Method
cpg	1577.82	J/mol×K	1270.69	Joback Method
cpg	1586.05	J/mol×K	1312.87	Joback Method
cpg	1592.51	J/mol×K	1355.05	Joback Method
dvisc	0.0002411	Pa×s	613.77	Joback Method

dvisc	0.0001172	Pa×s	695.14	Joback Method
dvisc	0.0000663	Pa×s	776.51	Joback Method
dvisc	0.0000418	Pa×s	857.88	Joback Method
dvisc	0.0000285	Pa×s	939.24	Joback Method
dvisc	0.0000207	Pa×s	1020.61	Joback Method
dvisc	0.0000157	Pa×s	1101.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382802&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