

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

Inchi:	InChI=1S/C30H46O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-24-33-29(31)27-21-16-17-22-28(29)
InchiKey:	VTGQPRNMRUIRGL-UHFFFAOYSA-N
Formula:	C30H46O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	470.68

Physical Properties

Property code	Value	Unit	Source
gf	-107.01	kJ/mol	Joback Method
hf	-823.84	kJ/mol	Joback Method
hfus	67.20	kJ/mol	Joback Method
hvap	103.37	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.599		Crippen Method
mvol	409.520	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	1079.10	K	Joback Method
tc	1323.82	K	Joback Method
tf	602.50	K	Joback Method
vc	1.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.95	J/molxK	1079.10	Joback Method
cpg	1478.29	J/molxK	1119.89	Joback Method
cpg	1492.55	J/molxK	1160.67	Joback Method
cpg	1504.84	J/molxK	1201.46	Joback Method
cpg	1515.24	J/molxK	1242.25	Joback Method
cpg	1523.85	J/molxK	1283.03	Joback Method
cpg	1530.77	J/molxK	1323.82	Joback Method
dvisc	0.0002741	Paxs	602.50	Joback Method

dvisc	0.0001344	Paxs	681.93	Joback Method
dvisc	0.0000765	Paxs	761.37	Joback Method
dvisc	0.0000484	Paxs	840.80	Joback Method
dvisc	0.0000332	Paxs	920.23	Joback Method
dvisc	0.0000241	Paxs	999.67	Joback Method
dvisc	0.0000184	Paxs	1079.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382801&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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