

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

Inchi:	InChI=1S/C28H42O4/c1-2-3-4-5-6-7-8-9-10-16-22-31-27(29)25-19-14-15-20-26(25)28(30)
InchiKey:	YTLIJTANWIJLSK-UHFFFAOYSA-N
Formula:	C28H42O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	442.63

Physical Properties

Property code	Value	Unit	Source
gf	-123.85	kJ/mol	Joback Method
hf	-782.56	kJ/mol	Joback Method
hfus	62.02	kJ/mol	Joback Method
hvap	98.92	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.819		Crippen Method
mcvol	381.340	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tb	1033.34	K	Joback Method
tc	1265.11	K	Joback Method
tf	579.96	K	Joback Method
vc	1.462	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.43	J/molxK	1033.34	Joback Method
cpg	1399.98	J/molxK	1226.48	Joback Method
cpg	1390.71	J/molxK	1187.85	Joback Method
cpg	1379.79	J/molxK	1149.23	Joback Method
cpg	1367.15	J/molxK	1110.60	Joback Method
cpg	1352.72	J/molxK	1071.97	Joback Method
cpg	1407.68	J/molxK	1265.11	Joback Method
dvisc	0.0000250	Paxs	1033.34	Joback Method

dvisc	0.0000326	Paxs	957.78	Joback Method
dvisc	0.0000446	Paxs	882.21	Joback Method
dvisc	0.0000646	Paxs	806.65	Joback Method
dvisc	0.0001011	Paxs	731.09	Joback Method
dvisc	0.0001756	Paxs	655.52	Joback Method
dvisc	0.0003519	Paxs	579.96	Joback Method

Sources

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=U382799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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