

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

Inchi:	InChI=1S/C24H34O4/c1-2-3-4-5-6-12-18-27-23(25)21-15-10-11-16-22(21)24(26)28-19-1
InchiKey:	VVIYFTUOVODATK-UHFFFAOYSA-N
Formula:	C24H34O4
SMILES:	CCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1cccc1
Mol. weight [g/mol]:	386.52

Physical Properties

Property code	Value	Unit	Source
gf	-157.53	kJ/mol	Joback Method
hf	-700.00	kJ/mol	Joback Method
hfus	51.66	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.258		Crippen Method
mvol	324.980	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2814.00		NIST Webbook
tb	941.82	K	Joback Method
tc	1160.54	K	Joback Method
tf	534.88	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.00	J/molxK	941.82	Joback Method
cpg	1105.43	J/molxK	978.27	Joback Method
cpg	1120.26	J/molxK	1014.73	Joback Method
cpg	1133.53	J/molxK	1051.18	Joback Method
cpg	1145.29	J/molxK	1087.63	Joback Method
cpg	1155.59	J/molxK	1124.09	Joback Method
cpg	1164.46	J/molxK	1160.54	Joback Method
dvisc	0.0005599	Paxs	534.88	Joback Method
dvisc	0.0002904	Paxs	602.70	Joback Method

dvisc	0.0001720	Paxs	670.53	Joback Method
dvisc	0.0001121	Paxs	738.35	Joback Method
dvisc	0.0000786	Paxs	806.17	Joback Method
dvisc	0.0000582	Paxs	874.00	Joback Method
dvisc	0.0000450	Paxs	941.82	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=U382795&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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