cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(phenethyl) ester

Inchi: InChI=1S/C24H26O4/c25-23(27-17-15-19-9-3-1-4-10-19)21-13-7-8-14-22(21)24(26)28-1

InchiKey: YCHDRXYELNNBCE-UHFFFAOYSA-N

Formula: C24H26O4

SMILES: O=C(OCCc1ccccc1)C1CC=CCC1C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	-45.12	kJ/mol	Joback Method
hf	-463.47	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	92.29	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.141		Crippen Method
mcvol	301.220	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2993.00		NIST Webbook
rinpol	2993.00		NIST Webbook
tb	968.50	K	Joback Method
tc	1209.18	K	Joback Method
tf	561.30	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.74	J/mol×K	968.50	Joback Method
cpg	998.80	J/mol×K	1008.61	Joback Method
cpg	1011.11	J/mol×K	1048.73	Joback Method
cpg	1021.75	J/mol×K	1088.84	Joback Method
cpg	1030.78	J/mol×K	1128.95	Joback Method
cpg	1038.27	J/mol×K	1169.07	Joback Method
cpg	1044.31	J/mol×K	1209.18	Joback Method
dvisc	0.0004965	Pa×s	561.30	Joback Method

dvisc	0.0002708	Pa×s	629.17	Joback Method
dvisc	0.0001662	Pa×s	697.03	Joback Method
dvisc	0.0001112	Pa×s	764.90	Joback Method
dvisc	0.0000795	Pa×s	832.77	Joback Method
dvisc	0.0000598	Pa×s	900.63	Joback Method
dvisc	0.0000467	Pa×s	968.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382803&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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