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

Inchi: InChI=1S/C19H24O4/c1-2-13-22-18(20)16-10-6-7-11-17(16)19(21)23-14-12-15-8-4-3-5-9

InchiKey: OBBNELHLXBIYHJ-UHFFFAOYSA-N

Formula: C19H24O4

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

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-199.63	kJ/mol	Joback Method
hf	-596.80	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.308		Crippen Method
mcvol	254.530	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2321.00		NIST Webbook
tb	827.42	K	Joback Method
tc	1048.85	K	Joback Method
tf	478.53	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.53	J/mol×K	827.42	Joback Method
cpg	807.29	J/mol×K	864.32	Joback Method
cpg	822.58	J/mol×K	901.23	Joback Method
cpg	836.43	J/mol×K	938.13	Joback Method
cpg	848.87	J/mol×K	975.04	Joback Method
cpg	859.93	J/mol×K	1011.94	Joback Method
cpg	869.64	J/mol×K	1048.85	Joback Method
dvisc	0.0009214	Pa×s	478.53	Joback Method
dvisc	0.0005056	Pa×s	536.68	Joback Method

dvisc	0.0003120	Pa×s	594.83	Joback Method
dvisc	0.0002098	Pa×s	652.98	Joback Method
dvisc	0.0001506	Pa×s	711.12	Joback Method
dvisc	0.0001136	Pa×s	769.27	Joback Method
dvisc	0.0000892	Pa×s	827.42	Joback Method

Sources

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=U382788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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