cis-Cyclohex-4-en-1,2-dicarboxylic acid, ethyl isohexyl ester

Inchi: InChI=1S/C16H26O4/c1-4-19-15(17)13-9-5-6-10-14(13)16(18)20-11-7-8-12(2)3/h5-6,12-

InchiKey: FQLHTDJFRLGLAW-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: CCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-339.74	kJ/mol	Joback Method
hf	-776.69	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.111		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1877.00		NIST Webbook
tb	731.66	K	Joback Method
tc	931.82	K	Joback Method
tf	403.30	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.67	J/mol×K	731.66	Joback Method
cpg	724.87	J/mol×K	765.02	Joback Method
cpg	741.91	J/mol×K	798.38	Joback Method
cpg	757.81	J/mol×K	831.74	Joback Method
cpg	772.57	J/mol×K	865.10	Joback Method
cpg	786.20	J/mol×K	898.46	Joback Method
cpg	798.70	J/mol×K	931.82	Joback Method
dvisc	0.0016405	Pa×s	403.30	Joback Method
dvisc	0.0008124	Pa×s	458.03	Joback Method

dvisc	0.0004674	Pa×s	512.75	Joback Method
dvisc	0.0002992	Pa×s	567.48	Joback Method
dvisc	0.0002071	Pa×s	622.21	Joback Method
dvisc	0.0001522	Pa×s	676.93	Joback Method
dvisc	0.0001171	Pa×s	731.66	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=U382681&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