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

Inchi: InChI=1S/C17H28O4/c1-4-11-20-16(18)14-9-7-8-10-15(14)17(19)21-12-13(5-2)6-3/h7-8,

InchiKey: JSOQUSBINRGBFO-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: CCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-331.32	kJ/mol	Joback Method
hf	-797.33	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	71.77	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.501		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	754.54	K	Joback Method
tc	953.24	K	Joback Method
tf	414.57	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.19	J/mol×K	754.54	Joback Method
cpg	782.54	J/mol×K	787.66	Joback Method
cpg	799.71	J/mol×K	820.77	Joback Method
cpg	815.69	J/mol×K	853.89	Joback Method
cpg	830.50	J/mol×K	887.00	Joback Method
cpg	844.16	J/mol×K	920.12	Joback Method
cpg	856.66	J/mol×K	953.24	Joback Method
dvisc	0.0015094	Pa×s	414.57	Joback Method

dvisc	0.0007381	Pa×s	471.23	Joback Method
dvisc	0.0004209	Pa×s	527.89	Joback Method
dvisc	0.0002676	Pa×s	584.56	Joback Method
dvisc	0.0001843	Pa×s	641.22	Joback Method
dvisc	0.0001349	Pa×s	697.88	Joback Method
dvisc	0.0001034	Pa×s	754.54	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=U382805&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