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

Inchi: InChI=1S/C18H30O4/c1-4-7-12-21-17(19)15-10-8-9-11-16(15)18(20)22-13-14(5-2)6-3/h8
InchiKey: PSAAZDDIHFLLQU-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: CCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-322.90	kJ/mol	Joback Method
hf	-817.97	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.891		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	777.42	K	Joback Method
tc	975.18	K	Joback Method
tf	425.84	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.66	J/mol×K	777.42	Joback Method
cpg	841.13	J/mol×K	810.38	Joback Method
cpg	858.38	J/mol×K	843.34	Joback Method
cpg	874.42	J/mol×K	876.30	Joback Method
cpg	889.25	J/mol×K	909.26	Joback Method
cpg	902.89	J/mol×K	942.22	Joback Method
cpg	915.36	J/mol×K	975.18	Joback Method
dvisc	0.0013807	Pa×s	425.84	Joback Method

dvisc	0.0006672	Pa×s	484.44	Joback Method
dvisc	0.0003772	Pa×s	543.03	Joback Method
dvisc	0.0002383	Pa×s	601.63	Joback Method
dvisc	0.0001633	Pa×s	660.23	Joback Method
dvisc	0.0001191	Pa×s	718.82	Joback Method
dvisc	0.0000910	Pa×s	777.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382806&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