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

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

Physical Properties

Property code	Value	Unit	Source
gf	-320.46	kJ/mol	Joback Method
hf	-812.69	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.036		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	777.86	K	Joback Method
tc	973.30	K	Joback Method
tf	440.84	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.16	J/mol×K	777.86	Joback Method
cpg	840.41	J/mol×K	810.43	Joback Method
cpg	857.48	J/mol×K	843.01	Joback Method
cpg	873.37	J/mol×K	875.58	Joback Method
cpg	888.09	J/mol×K	908.15	Joback Method
cpg	901.66	J/mol×K	940.73	Joback Method
cpg	914.09	J/mol×K	973.30	Joback Method
dvisc	0.0011808	Pa×s	440.84	Joback Method

dvisc	0.0006185	Pa×s	497.01	Joback Method
dvisc	0.0003694	Pa×s	553.18	Joback Method
dvisc	0.0002426	Pa×s	609.35	Joback Method
dvisc	0.0001711	Pa×s	665.52	Joback Method
dvisc	0.0001274	Pa×s	721.69	Joback Method
dvisc	0.0000989	Pa×s	777.86	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=U382661&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