1,2-Cyclohexanedicarboxylic acid, butyl isobutyl ester

Inchi: InChI=1S/C16H28O4/c1-4-5-10-19-15(17)13-8-6-7-9-14(13)16(18)20-11-12(2)3/h12-14H
InchiKey: HYXGOZPSEVFYHG-UHFFFAOYSA-N
Formula: C16H28O4
SMILES: CCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-369.70	kJ/mol	Joback Method
hf	-834.47	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	69.25	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.335		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	732.50	K	Joback Method
tc	931.39	K	Joback Method
tf	402.54	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.91	J/mol×K	732.50	Joback Method
cpg	815.32	J/mol×K	898.24	Joback Method
cpg	800.99	J/mol×K	865.09	Joback Method
cpg	785.49	J/mol×K	831.94	Joback Method
cpg	768.81	J/mol×K	798.80	Joback Method
cpg	750.96	J/mol×K	765.65	Joback Method
cpg	828.49	J/mol×K	931.39	Joback Method
dvisc	0.0001105	Pa×s	732.50	Joback Method

dvisc	0.0001453	Pa×s	677.51	Joback Method
dvisc	0.0002004	Pa×s	622.51	Joback Method
dvisc	0.0002943	Pa×s	567.52	Joback Method
dvisc	0.0004693	Pa×s	512.53	Joback Method
dvisc	0.0008371	Pa×s	457.53	Joback Method
dvisc	0.0017491	Pa×s	402.54	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=U339439&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