1,2-Cyclohexanedicarboxylic acid, di(3-methylbut-2-yl) ester

Inchi: InChI=1S/C18H32O4/c1-11(2)13(5)21-17(19)15-9-7-8-10-16(15)18(20)22-14(6)12(3)4/h1

InchiKey: RMIWZZXXPRWNSX-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CC(C)C(C)OC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-360.18	kJ/mol	Joback Method
hf	-891.59	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	72.54	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.968		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
tb	776.94	K	Joback Method
tc	981.30	K	Joback Method
tf	380.08	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.71	J/mol×K	776.94	Joback Method
cpg	937.03	J/mol×K	947.24	Joback Method
cpg	922.51	J/mol×K	913.18	Joback Method
cpg	906.63	J/mol×K	879.12	Joback Method
cpg	889.38	J/mol×K	845.06	Joback Method
cpg	870.74	J/mol×K	811.00	Joback Method
cpg	950.22	J/mol×K	981.30	Joback Method
dvisc	0.0000663	Pa×s	776.94	Joback Method

dvisc	0.0000924	Pa×s	710.80	Joback Method
dvisc	0.0001379	Pa×s	644.65	Joback Method
dvisc	0.0002254	Pa×s	578.51	Joback Method
dvisc	0.0004181	Pa×s	512.37	Joback Method
dvisc	0.0009317	Pa×s	446.22	Joback Method
dvisc	0.0027441	Pa×s	380.08	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=U339571&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