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

Inchi: InChI=1S/C20H36O4/c1-7-17(13(3)4)23-19(21)15-11-9-10-12-16(15)20(22)24-18(8-2)14

InchiKey: RGQKNUDLRLDOKP-UHFFFAOYSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-343.34	kJ/mol	Joback Method
hf	-932.87	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.748		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	822.70	K	Joback Method
tc	1025.44	K	Joback Method
tf	402.62	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.41	J/mol×K	822.70	Joback Method
cpg	1056.78	J/mol×K	991.65	Joback Method
cpg	1042.56	J/mol×K	957.86	Joback Method
cpg	1026.93	J/mol×K	924.07	Joback Method
cpg	1009.88	J/mol×K	890.28	Joback Method
cpg	991.37	J/mol×K	856.49	Joback Method
cpg	1069.60	J/mol×K	1025.44	Joback Method
dvisc	0.0000501	Pa×s	822.70	Joback Method

dvisc	0.0000700	Pa×s	752.69	Joback Method
dvisc	0.0001047	Pa×s	682.67	Joback Method
dvisc	0.0001718	Pa×s	612.66	Joback Method
dvisc	0.0003203	Pa×s	542.65	Joback Method
dvisc	0.0007181	Pa×s	472.63	Joback Method
dvisc	0.0021323	Pa×s	402.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339452&Units=SI
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

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