cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(2-methylpent-3-yl) ester

Inchi: InChI=1S/C20H34O4/c1-7-17(13(3)4)23-19(21)15-11-9-10-12-16(15)20(22)24-18(8-2)14

InchiKey: YATYGCAZZLBGLV-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCC(OC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C)C(C)C

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-313.38	kJ/mol	Joback Method
hf	-875.09	kJ/mol	Joback Method
hfus	33.17	kJ/mol	Joback Method
hvap	77.29	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.524		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	821.86	K	Joback Method
tc	1025.52	K	Joback Method
tf	403.38	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.57	J/mol×K	821.86	Joback Method
cpg	962.79	J/mol×K	855.80	Joback Method
cpg	980.58	J/mol×K	889.75	Joback Method
cpg	996.96	J/mol×K	923.69	Joback Method
cpg	1011.96	J/mol×K	957.64	Joback Method
cpg	1025.60	J/mol×K	991.58	Joback Method
cpg	1037.89	J/mol×K	1025.52	Joback Method
dvisc	0.0019978	Pa×s	403.38	Joback Method

dvisc	0.0007019	Pa×s	473.13	Joback Method
dvisc	0.0003226	Pa×s	542.87	Joback Method
dvisc	0.0001770	Pa×s	612.62	Joback Method
dvisc	0.0001098	Pa×s	682.37	Joback Method
dvisc	0.0000744	Pa×s	752.11	Joback Method
dvisc	0.0000539	Pa×s	821.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382770&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