1,2-Cyclohexanedicarboxylic acid, hexyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C20H36O4/c1-5-7-8-11-14-23-19(21)16-12-9-10-13-17(16)20(22)24-18(6-2)15

InchiKey: FXKITTJOEFEUKD-UHFFFAOYSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-338.46	kJ/mol	Joback Method
hf	-922.31	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	77.77	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.894		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	823.58	K	Joback Method
tc	1022.33	K	Joback Method
tf	432.62	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.46	J/mol×K	823.58	Joback Method
cpg	990.04	J/mol×K	856.70	Joback Method
cpg	1008.24	J/mol×K	889.83	Joback Method
cpg	1025.07	J/mol×K	922.95	Joback Method
cpg	1040.54	J/mol×K	956.08	Joback Method
cpg	1054.67	J/mol×K	989.20	Joback Method
cpg	1067.49	J/mol×K	1022.33	Joback Method
dvisc	0.0014062	Pa×s	432.62	Joback Method

dvisc	0.0005879	Pa×s	497.78	Joback Method
dvisc	0.0003007	Pa×s	562.94	Joback Method
dvisc	0.0001768	Pa×s	628.10	Joback Method
dvisc	0.0001149	Pa×s	693.26	Joback Method
dvisc	0.0000804	Pa×s	758.42	Joback Method
dvisc	0.0000595	Pa×s	823.58	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=U339443&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