

1,2-Cyclohexanedicarboxylic acid, dihexyl ester

Inchi:	InChI=1S/C20H36O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6
InchiKey:	HCWCRSSMHYWRGG-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-333.58	kJ/mol	Joback Method
hf	-911.75	kJ/mol	Joback Method
hfus	46.04	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	5.040		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	824.46	K	Joback Method
tc	1019.78	K	Joback Method
tf	462.62	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.51	J/molxK	824.46	Joback Method
cpg	988.77	J/molxK	857.01	Joback Method
cpg	1006.70	J/molxK	889.57	Joback Method
cpg	1023.33	J/molxK	922.12	Joback Method
cpg	1038.67	J/molxK	954.67	Joback Method
cpg	1052.74	J/molxK	987.22	Joback Method
cpg	1065.56	J/molxK	1019.78	Joback Method
dvisc	0.0010134	Paxs	462.62	Joback Method

dvisc	0.0005034	Paxs	522.93	Joback Method
dvisc	0.0002890	Paxs	583.23	Joback Method
dvisc	0.0001841	Paxs	643.54	Joback Method
dvisc	0.0001267	Paxs	703.85	Joback Method
dvisc	0.0000925	Paxs	764.15	Joback Method
dvisc	0.0000707	Paxs	824.46	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=U339411&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

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