

1,2-Cyclohexanedicarboxylic acid, cyclohexyl isohexyl ester

Inchi:	InChI=1S/C20H34O4/c1-15(2)9-8-14-23-19(21)17-12-6-7-13-18(17)20(22)24-16-10-4-3-5
InchiKey:	JWSKCIXLDHKWKV-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	CC(C)CCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-311.57	kJ/mol	Joback Method
hf	-862.71	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	78.59	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.648		Crippen Method
mvol	285.820	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	843.57	K	Joback Method
tc	1060.05	K	Joback Method
tf	455.00	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.21	J/molxK	843.57	Joback Method
cpg	1052.39	J/molxK	1023.97	Joback Method
cpg	1038.78	J/molxK	987.89	Joback Method
cpg	1023.49	J/molxK	951.81	Joback Method
cpg	1006.48	J/molxK	915.73	Joback Method
cpg	987.73	J/molxK	879.65	Joback Method
cpg	1064.33	J/molxK	1060.05	Joback Method
dvisc	0.0000672	Paxs	843.57	Joback Method

dvisc	0.0000901	Paxs	778.81	Joback Method
dvisc	0.0001273	Paxs	714.05	Joback Method
dvisc	0.0001928	Paxs	649.28	Joback Method
dvisc	0.0003199	Paxs	584.52	Joback Method
dvisc	0.0006024	Paxs	519.76	Joback Method
dvisc	0.0013583	Paxs	455.00	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=U339762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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