1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl pentyl ester

Inchi: InChI=1S/C20H34O4/c1-2-3-9-14-23-19(21)17-12-7-8-13-18(17)20(22)24-15-16-10-5-4-6

InchiKey: WDTGTPBLLDQGHP-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-309.13	kJ/mol	Joback Method
hf	-857.43	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.650		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	844.01	K	Joback Method
tc	1057.86	K	Joback Method
tf	470.00	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/mol×K	844.01	Joback Method
cpg	987.02	J/mol×K	879.65	Joback Method
cpg	1005.59	J/mol×K	915.29	Joback Method
cpg	1022.47	J/mol×K	950.94	Joback Method
cpg	1037.69	J/mol×K	986.58	Joback Method
cpg	1051.27	J/mol×K	1022.22	Joback Method
cpg	1063.24	J/mol×K	1057.86	Joback Method
dvisc	0.0011636	Pa×s	470.00	Joback Method

dvisc	0.0005606	Pa×s	532.34	Joback Method
dvisc	0.0003148	Pa×s	594.67	Joback Method
dvisc	0.0001972	Pa×s	657.00	Joback Method
dvisc	0.0001340	Pa×s	719.34	Joback Method
dvisc	0.0000968	Pa×s	781.67	Joback Method
dvisc	0.0000734	Pa×s	844.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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