1,2-Cyclohexanedicarboxylic acid, heptyl pentyl ester

Inchi: InChI=1S/C20H36O4/c1-3-5-7-8-12-16-24-20(22)18-14-10-9-13-17(18)19(21)23-15-11-6

InchiKey: QDFABZWRLYBOFO-UHFFFAOYSA-N

Formula: C20H36O4

SMILES: CCCCCCCOC(=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
mcvol	296.680	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	824.46	K	Joback Method
tc	1019.78	K	Joback Method
tf	462.62	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005034	Pa×s	522.93	Joback Method
dvisc	0.0002890	Pa×s	583.23	Joback Method
dvisc	0.0001841	Pa×s	643.54	Joback Method
dvisc	0.0001267	Pa×s	703.85	Joback Method
dvisc	0.0000925	Pa×s	764.15	Joback Method
dvisc	0.0000707	Pa×s	824.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339470&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

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