1,2-Cyclohexanedicarboxylic acid, octyl pentyl ester

Inchi: InChI=1S/C21H38O4/c1-3-5-7-8-9-13-17-25-21(23)19-15-11-10-14-18(19)20(22)24-16-1

InchiKey: IXYWJHRZBYPXDE-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-325.16	kJ/mol	Joback Method
hf	-932.39	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.430		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2430.00		NIST Webbook
tb	847.34	K	Joback Method
tc	1044.08	K	Joback Method
tf	473.89	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.95	J/mol×K	847.34	Joback Method
cpg	1050.31	J/mol×K	880.13	Joback Method
cpg	1068.30	J/mol×K	912.92	Joback Method
cpg	1084.92	J/mol×K	945.71	Joback Method
cpg	1100.21	J/mol×K	978.50	Joback Method
cpg	1114.17	J/mol×K	1011.29	Joback Method
cpg	1126.84	J/mol×K	1044.08	Joback Method
dvisc	0.0009131	Pa×s	473.89	Joback Method
dvisc	0.0004486	Pa×s	536.13	Joback Method

dvisc	0.0002555	Pa×s	598.37	Joback Method
dvisc	0.0001618	Pa×s	660.62	Joback Method
dvisc	0.0001109	Pa×s	722.86	Joback Method
dvisc	0.0000807	Pa×s	785.10	Joback Method
dvisc	0.0000615	Pa×s	847.34	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=U339471&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