1,2-Cyclohexanedicarboxylic acid, 4-octyl pentyl ester

Inchi: InChI=1S/C21H38O4/c1-4-7-11-16-24-20(22)18-14-9-10-15-19(18)21(23)25-17(12-6-3)1

InchiKey: MZERJONFDDDGNE-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-327.60	kJ/mol	Joback Method
hf	-937.67	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.428		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	846.90	K	Joback Method
tc	1044.97	K	Joback Method
tf	458.89	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.42	J/mol×K	846.90	Joback Method
cpg	1114.96	J/mol×K	1011.96	Joback Method
cpg	1100.98	J/mol×K	978.95	Joback Method
cpg	1085.66	J/mol×K	945.93	Joback Method
cpg	1068.97	J/mol×K	912.92	Joback Method
cpg	1050.90	J/mol×K	879.91	Joback Method
cpg	1127.60	J/mol×K	1044.97	Joback Method
dvisc	0.0000563	Pa×s	846.90	Joback Method

dvisc	0.0000751	Pa×s	782.23	Joback Method
dvisc	0.0001053	Pa×s	717.56	Joback Method
dvisc	0.0001580	Pa×s	652.89	Joback Method
dvisc	0.0002591	Pa×s	588.23	Joback Method
dvisc	0.0004803	Pa×s	523.56	Joback Method
dvisc	0.0010593	Pa×s	458.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339519&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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