1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl pentyl ester

Inchi: InChI=1S/C21H36O4/c1-2-3-9-15-24-20(22)18-12-7-8-13-19(18)21(23)25-16-14-17-10-5

InchiKey: MWJWABNRDZWNJJ-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-300.71	kJ/mol	Joback Method
hf	-878.07	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	81.20	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.040		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	2497.00		NIST Webbook
tb	866.89	K	Joback Method
tc	1079.98	K	Joback Method
tf	481.27	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.27	J/mol×K	866.89	Joback Method
cpg	1048.33	J/mol×K	902.40	Joback Method
cpg	1066.65	J/mol×K	937.92	Joback Method
cpg	1083.26	J/mol×K	973.43	Joback Method
cpg	1098.19	J/mol×K	1008.95	Joback Method
cpg	1111.46	J/mol×K	1044.46	Joback Method
cpg	1123.10	J/mol×K	1079.98	Joback Method
dvisc	0.0010437	Pa×s	481.27	Joback Method
dvisc	0.0004977	Pa×s	545.54	Joback Method

dvisc	0.0002774	Pa×s	609.81	Joback Method
dvisc	0.0001729	Pa×s	674.08	Joback Method
dvisc	0.0001170	Pa×s	738.35	Joback Method
dvisc	0.0000842	Pa×s	802.62	Joback Method
dvisc	0.0000637	Pa×s	866.89	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=U339726&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