1,2-Cyclohexanedicarboxylic acid, hexyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C21H36O4/c1-3-4-5-10-15-24-20(22)17-12-7-8-13-18(17)21(23)25-19-14-9-6-1

InchiKey: PHLSWPQPIQIRCK-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-308.42	kJ/mol	Joback Method
hf	-898.41	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.038		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	862.22	K	Joback Method
tc	1075.00	K	Joback Method
tf	477.03	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.72	J/mol×K	862.22	Joback Method
cpg	1116.31	J/mol×K	1039.53	Joback Method
cpg	1102.90	J/mol×K	1004.07	Joback Method
cpg	1087.75	J/mol×K	968.61	Joback Method
cpg	1070.85	J/mol×K	933.15	Joback Method
cpg	1052.18	J/mol×K	897.68	Joback Method
cpg	1128.02	J/mol×K	1075.00	Joback Method
dvisc	0.0000827	Pa×s	862.22	Joback Method

dvisc	0.0001071	Pa×s	798.02	Joback Method
dvisc	0.0001453	Pa×s	733.82	Joback Method
dvisc	0.0002088	Pa×s	669.62	Joback Method
dvisc	0.0003242	Pa×s	605.43	Joback Method
dvisc	0.0005586	Pa×s	541.23	Joback Method
dvisc	0.0011145	Pa×s	477.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339880&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