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

Inchi: InChI=1S/C20H34O4/c1-3-4-9-14-23-19(21)16-11-6-7-12-17(16)20(22)24-18-13-8-5-10-1

InchiKey: QGIGGZWIUSLYMU-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-316.84	kJ/mol	Joback Method
hf	-877.77	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.648		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	839.34	K	Joback Method
tc	1052.96	K	Joback Method
tf	465.76	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.02	J/mol×K	839.34	Joback Method
cpg	1056.16	J/mol×K	1017.36	Joback Method
cpg	1042.38	J/mol×K	981.76	Joback Method
cpg	1026.89	J/mol×K	946.15	Joback Method
cpg	1009.68	J/mol×K	910.55	Joback Method
cpg	990.73	J/mol×K	874.94	Joback Method
cpg	1068.25	J/mol×K	1052.96	Joback Method
dvisc	0.0000945	Pa×s	839.34	Joback Method

dvisc	0.0001221	Pa×s	777.08	Joback Method
dvisc	0.0001650	Pa×s	714.81	Joback Method
dvisc	0.0002361	Pa×s	652.55	Joback Method
dvisc	0.0003643	Pa×s	590.29	Joback Method
dvisc	0.0006226	Pa×s	528.02	Joback Method
dvisc	0.0012281	Pa×s	465.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339878&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