1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl octyl ester

Inchi: InChI=1S/C22H40O4/c1-5-7-8-9-10-13-16-25-21(23)18-14-11-12-15-19(18)22(24)26-20(

InchiKey: RERMIMVIRVCJOM-UHFFFAOYSA-N

Formula: C22H40O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-321.62	kJ/mol	Joback Method
hf	-963.59	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	82.22	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.674		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	869.34	K	Joback Method
tc	1070.39	K	Joback Method
tf	455.16	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.91	J/mol×K	869.34	Joback Method
cpg	1113.57	J/mol×K	902.85	Joback Method
cpg	1131.72	J/mol×K	936.36	Joback Method
cpg	1148.41	J/mol×K	969.87	Joback Method
cpg	1163.65	J/mol×K	1003.38	Joback Method
cpg	1177.46	J/mol×K	1036.88	Joback Method
cpg	1189.87	J/mol×K	1070.39	Joback Method
dvisc	0.0011117	Pa×s	455.16	Joback Method

dvisc	0.0004572	Pa×s	524.19	Joback Method
dvisc	0.0002313	Pa×s	593.22	Joback Method
dvisc	0.0001348	Pa×s	662.25	Joback Method
dvisc	0.0000870	Pa×s	731.28	Joback Method
dvisc	0.0000606	Pa×s	800.31	Joback Method
dvisc	0.0000447	Pa×s	869.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339445&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