cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-methylpent-3-yl octyl ester

Inchi: InChI=1S/C22H38O4/c1-5-7-8-9-10-13-16-25-21(23)18-14-11-12-15-19(18)22(24)26-20(

InchiKey: KHDRGOLRFVGAOF-UHFFFAOYSA-N

Formula: C22H38O4

SMILES: CCCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-291.66	kJ/mol	Joback Method
hf	-905.81	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	82.51	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.450		Crippen Method
mcvol	320.560	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	868.50	K	Joback Method
tc	1070.02	K	Joback Method
tf	455.92	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.89	J/mol×K	868.50	Joback Method
cpg	1083.83	J/mol×K	902.09	Joback Method
cpg	1101.33	J/mol×K	935.67	Joback Method
cpg	1117.40	J/mol×K	969.26	Joback Method
cpg	1132.07	J/mol×K	1002.85	Joback Method
cpg	1145.36	J/mol×K	1036.44	Joback Method
cpg	1157.31	J/mol×K	1070.02	Joback Method
dvisc	0.0010737	Pa×s	455.92	Joback Method

dvisc	0.0004565	Pa×s	524.68	Joback Method
dvisc	0.0002367	Pa×s	593.45	Joback Method
dvisc	0.0001406	Pa×s	662.21	Joback Method
dvisc	0.0000922	Pa×s	730.97	Joback Method
dvisc	0.0000649	Pa×s	799.74	Joback Method
dvisc	0.0000484	Pa×s	868.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382765&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

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