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

Inchi: InChI=1S/C21H36O4/c1-5-7-8-9-12-15-24-20(22)17-13-10-11-14-18(17)21(23)25-19(6-2
InchiKey: DLQKXNNBJYGGBC-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: CCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-300.08	kJ/mol	Joback Method
hf	-885.17	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	80.29	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.060		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	845.62	K	Joback Method
tc	1045.79	K	Joback Method
tf	444.65	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.43	J/mol×K	845.62	Joback Method
cpg	1022.31	J/mol×K	878.98	Joback Method
cpg	1039.81	J/mol×K	912.34	Joback Method
cpg	1055.93	J/mol×K	945.70	Joback Method
cpg	1070.70	J/mol×K	979.06	Joback Method
cpg	1084.14	J/mol×K	1012.42	Joback Method
cpg	1096.27	J/mol×K	1045.79	Joback Method
dvisc	0.0012029	Pa×s	444.65	Joback Method

dvisc	0.0005159	Pa×s	511.48	Joback Method
dvisc	0.0002691	Pa×s	578.31	Joback Method
dvisc	0.0001606	Pa×s	645.13	Joback Method
dvisc	0.0001056	Pa×s	711.96	Joback Method
dvisc	0.0000746	Pa×s	778.79	Joback Method
dvisc	0.0000557	Pa×s	845.62	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=U382764&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