1,2-Cyclohexanedicarboxylic acid, cyclohex-3-enylmethyl hexyl ester

Inchi: InChI=1S/C21H34O4/c1-2-3-4-10-15-24-20(22)18-13-8-9-14-19(18)21(23)25-16-17-11-6

InchiKey: GQFLOEOTHCQOOA-UHFFFAOYSA-N

Formula: C21H34O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-270.75	kJ/mol	Joback Method
hf	-820.29	kJ/mol	Joback Method
hfus	41.68	kJ/mol	Joback Method
hvap	81.49	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.816		Crippen Method
mcvol	295.610	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	866.05	K	Joback Method
tc	1080.10	K	Joback Method
tf	482.03	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.32	J/mol×K	866.05	Joback Method
cpg	1079.40	J/mol×K	1044.42	Joback Method
cpg	1066.66	J/mol×K	1008.75	Joback Method
cpg	1052.31	J/mol×K	973.07	Joback Method
cpg	1036.32	J/mol×K	937.40	Joback Method
cpg	1018.67	J/mol×K	901.72	Joback Method
cpg	1090.56	J/mol×K	1080.10	Joback Method
dvisc	0.0000690	Pa×s	866.05	Joback Method

dvisc	0.0000903	Pa×s	802.05	Joback Method
dvisc	0.0001240	Pa×s	738.04	Joback Method
dvisc	0.0001807	Pa×s	674.04	Joback Method
dvisc	0.0002851	Pa×s	610.04	Joback Method
dvisc	0.0005006	Pa×s	546.03	Joback Method
dvisc	0.0010206	Pa×s	482.03	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=U339871&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