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

Inchi: InChI=1S/C21H34O4/c1-16(2)9-8-14-24-20(22)18-12-6-7-13-19(18)21(23)25-15-17-10-4

InchiKey: NUVAWUAGVVGSBE-UHFFFAOYSA-N

Formula: C21H34O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-273.19	kJ/mol	Joback Method
hf	-825.57	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.672		Crippen Method
mcvol	295.610	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook
tb	865.61	K	Joback Method
tc	1082.03	K	Joback Method
tf	467.03	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.80	J/mol×K	865.61	Joback Method
cpg	1080.35	J/mol×K	1045.96	Joback Method
cpg	1067.61	J/mol×K	1009.89	Joback Method
cpg	1053.21	J/mol×K	973.82	Joback Method
cpg	1037.13	J/mol×K	937.75	Joback Method
cpg	1019.33	J/mol×K	901.68	Joback Method
cpg	1091.46	J/mol×K	1082.03	Joback Method
dvisc	0.0000631	Pa×s	865.61	Joback Method

dvisc	0.0000839	Pa×s	799.18	Joback Method
dvisc	0.0001175	Pa×s	732.75	Joback Method
dvisc	0.0001759	Pa×s	666.32	Joback Method
dvisc	0.0002881	Pa×s	599.89	Joback Method
dvisc	0.0005334	Pa×s	533.46	Joback Method
dvisc	0.0011766	Pa×s	467.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339870&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