1,2-Cyclohexanedicarboxylic acid, di(cyclohex-3-enylmethyl) ester

Inchi: InChI=1S/C22H32O4/c23-21(25-15-17-9-3-1-4-10-17)19-13-7-8-14-20(19)22(24)26-16-1

InchiKey: GNXFGKUPZDWEOT-UHFFFAOYSA-N

Formula: C22H32O4

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

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-207.92	kJ/mol	Joback Method
hf	-728.83	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.592		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	907.64	K	Joback Method
tc	1144.21	K	Joback Method
tf	501.44	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.33	J/mol×K	907.64	Joback Method
cpg	1101.52	J/mol×K	1104.78	Joback Method
cpg	1090.84	J/mol×K	1065.36	Joback Method
cpg	1078.14	J/mol×K	1025.93	Joback Method
cpg	1063.35	J/mol×K	986.50	Joback Method
cpg	1046.43	J/mol×K	947.07	Joback Method
cpg	1110.20	J/mol×K	1144.21	Joback Method
dvisc	0.0000673	Pa×s	907.64	Joback Method

dvisc	0.0000883	Pa×s	839.94	Joback Method
dvisc	0.0001214	Pa×s	772.24	Joback Method
dvisc	0.0001775	Pa×s	704.54	Joback Method
dvisc	0.0002813	Pa×s	636.84	Joback Method
dvisc	0.0004975	Pa×s	569.14	Joback Method
dvisc	0.0010263	Pa×s	501.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339875&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