1,2-Cyclohexanedicarboxylic acid, 2-ethoxyethyl nonyl ester

Inchi: InChI=1S/C21H38O5/c1-3-5-6-7-8-9-12-15-25-20(22)18-13-10-11-14-19(18)21(23)26-17
InchiKey: BTTJSVRNGQSAGU-UHFFFAOYSA-N
Formula: C21H38O5
SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC
Mol. weight [g/mol]: 370.52

Physical Properties

Property code	Value	Unit	Source
gf	-430.16	kJ/mol	Joback Method
hf	-1064.61	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.666		Crippen Method
mcvol	316.640	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	869.76	K	Joback Method
tc	1068.88	K	Joback Method
tf	496.12	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.78	J/mol×K	869.76	Joback Method
cpg	1081.56	J/mol×K	902.95	Joback Method
cpg	1098.86	J/mol×K	936.13	Joback Method
cpg	1114.68	J/mol×K	969.32	Joback Method
cpg	1129.04	J/mol×K	1002.50	Joback Method
cpg	1141.95	J/mol×K	1035.69	Joback Method
cpg	1153.41	J/mol×K	1068.88	Joback Method
dvisc	0.0006307	Pa×s	496.12	Joback Method

dvisc	0.0003197	Pa×s	558.39	Joback Method
dvisc	0.0001857	Pa×s	620.67	Joback Method
dvisc	0.0001191	Pa×s	682.94	Joback Method
dvisc	0.0000823	Pa×s	745.21	Joback Method
dvisc	0.0000602	Pa×s	807.49	Joback Method
dvisc	0.0000460	Pa×s	869.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339911&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