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

Inchi: InChI=1S/C23H42O5/c1-3-5-6-7-8-9-10-11-14-17-27-22(24)20-15-12-13-16-21(20)23(25
InchiKey: JQIXMXPOTVXORM-UHFFFAOYSA-N
Formula: C23H42O5
SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC
Mol. weight [g/mol]: 398.58

Physical Properties

Property code	Value	Unit	Source
gf	-413.32	kJ/mol	Joback Method
hf	-1105.89	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.447		Crippen Method
mcvol	344.820	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	915.52	K	Joback Method
tc	1121.29	K	Joback Method
tf	518.66	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.49	J/mol×K	915.52	Joback Method
cpg	1206.45	J/mol×K	949.81	Joback Method
cpg	1223.74	J/mol×K	984.11	Joback Method
cpg	1239.38	J/mol×K	1018.40	Joback Method
cpg	1253.39	J/mol×K	1052.70	Joback Method
cpg	1265.78	J/mol×K	1086.99	Joback Method
cpg	1276.57	J/mol×K	1121.29	Joback Method
dvisc	0.0005027	Pa×s	518.66	Joback Method

dvisc	0.0002496	Pa×s	584.80	Joback Method
dvisc	0.0001428	Pa×s	650.95	Joback Method
dvisc	0.0000906	Pa×s	717.09	Joback Method
dvisc	0.0000621	Pa×s	783.23	Joback Method
dvisc	0.0000451	Pa×s	849.38	Joback Method
dvisc	0.0000343	Pa×s	915.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339913&Units=SI

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