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

Inchi: InChI=1S/C22H40O5/c1-3-5-6-7-8-9-10-13-16-26-21(23)19-14-11-12-15-20(19)22(24)27
InchiKey: HCXGDTBLFYGQMQ-UHFFFAOYSA-N
Formula: C22H40O5
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC
Mol. weight [g/mol]: 384.55

Physical Properties

Property code	Value	Unit	Source
gf	-421.74	kJ/mol	Joback Method
hf	-1085.25	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	85.41	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.056		Crippen Method
mcvol	330.730	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	892.64	K	Joback Method
tc	1094.65	K	Joback Method
tf	507.39	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.90	J/mol×K	892.64	Joback Method
cpg	1143.76	J/mol×K	926.31	Joback Method
cpg	1161.06	J/mol×K	959.98	Joback Method
cpg	1176.80	J/mol×K	993.64	Joback Method
cpg	1191.00	J/mol×K	1027.31	Joback Method
cpg	1203.67	J/mol×K	1060.98	Joback Method
cpg	1214.82	J/mol×K	1094.65	Joback Method
dvisc	0.0005641	Pa×s	507.39	Joback Method

dvisc	0.0002829	Pa×s	571.60	Joback Method
dvisc	0.0001631	Pa×s	635.81	Joback Method
dvisc	0.0001040	Pa×s	700.01	Joback Method
dvisc	0.0000716	Pa×s	764.22	Joback Method
dvisc	0.0000522	Pa×s	828.43	Joback Method
dvisc	0.0000398	Pa×s	892.64	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=U339912&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

Latest version available from:
https://www.chemeo.com/cid/86-867-5/1-2-Cyclohexanedicarboxylic-acid-decyl-2-ethoxyethyl-ester.pdf
Generated by Cheméo on 2024-04-27 19:24:26.863798067 +0000 UTC m=+16535115.784375383.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.