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

Inchi: InChI=1S/C29H54O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-33-28(30)26-21-18

InchiKey: YXWVBYIQQBTFHS-UHFFFAOYSA-N

Formula: C29H54O5

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC

Mol. weight [g/mol]: 482.74

Physical Properties

Property code	Value	Unit	Source
gf	-362.80	kJ/mol	Joback Method
hf	-1229.73	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	100.99	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.787		Crippen Method
mcvol	429.360	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	3321.00		NIST Webbook
tb	1052.80	K	Joback Method
tc	1303.51	K	Joback Method
tf	586.28	K	Joback Method
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1569.61	J/mol×K	1052.80	Joback Method
cpg	1589.34	J/mol×K	1094.58	Joback Method
cpg	1606.36	J/mol×K	1136.37	Joback Method
cpg	1620.75	J/mol×K	1178.15	Joback Method
cpg	1632.55	J/mol×K	1219.94	Joback Method
cpg	1641.83	J/mol×K	1261.72	Joback Method
cpg	1648.65	J/mol×K	1303.51	Joback Method
dvisc	0.0002368	Pa×s	586.28	Joback Method
dvisc	0.0001114	Pa×s	664.03	Joback Method

dvisc	0.0000614	Pa×s	741.79	Joback Method
dvisc	0.0000379	Pa×s	819.54	Joback Method
dvisc	0.0000254	Pa×s	897.29	Joback Method
dvisc	0.0000182	Pa×s	975.05	Joback Method
dvisc	0.0000136	Pa×s	1052.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339918&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