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

Inchi: InChI=1S/C28H52O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-22-32-27(29)25-20-17-18

InchiKey: BWZTXNJZQAWLBG-UHFFFAOYSA-N

Formula: C28H52O5

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

Mol. weight [g/mol]: 468.71

Physical Properties

Property code	Value	Unit	Source
gf	-371.22	kJ/mol	Joback Method
hf	-1209.09	kJ/mol	Joback Method
hfus	67.94	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.397		Crippen Method
mcvol	415.270	ml/mol	McGowan Method
pc	746.92	kPa	Joback Method
rinpol	3215.00		NIST Webbook
rinpol	3215.00		NIST Webbook
tb	1029.92	K	Joback Method
tc	1270.06	K	Joback Method
tf	575.01	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1505.42	J/mol×K	1029.92	Joback Method
cpg	1525.00	J/mol×K	1069.94	Joback Method
cpg	1542.13	J/mol×K	1109.97	Joback Method
cpg	1556.85	J/mol×K	1149.99	Joback Method
cpg	1569.20	J/mol×K	1190.01	Joback Method
cpg	1579.24	J/mol×K	1230.04	Joback Method
cpg	1587.01	J/mol×K	1270.06	Joback Method
dvisc	0.0002702	Pa×s	575.01	Joback Method

dvisc	0.0001281	Pa×s	650.83	Joback Method
dvisc	0.0000710	Pa×s	726.65	Joback Method
dvisc	0.0000440	Pa×s	802.47	Joback Method
dvisc	0.0000296	Pa×s	878.28	Joback Method
dvisc	0.0000212	Pa×s	954.10	Joback Method
dvisc	0.0000160	Pa×s	1029.92	Joback Method

Sources

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=U339917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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