1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl dodecyl ester

Inchi: InChI=1S/C28H50O4/c1-2-3-4-5-6-7-8-9-10-16-22-31-27(29)25-19-14-15-20-26(25)28(30

InchiKey: NGEAJBDVYIQVRX-UHFFFAOYSA-N

Formula: C28H50O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-241.77	kJ/mol	Joback Method
hf	-1022.55	kJ/mol	Joback Method
hfus	58.59	kJ/mol	Joback Method
hvap	96.78	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.771		Crippen Method
mcvol	398.540	ml/mol	McGowan Method
pc	846.53	kPa	Joback Method
rinpol	3224.00		NIST Webbook
rinpol	3224.00		NIST Webbook
tb	1027.05	K	Joback Method
tc	1257.68	K	Joback Method
tf	560.16	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1470.35	J/mol×K	1027.05	Joback Method
cpg	1542.86	J/mol×K	1219.24	Joback Method
cpg	1532.56	J/mol×K	1180.80	Joback Method
cpg	1520.22	J/mol×K	1142.36	Joback Method
cpg	1505.79	J/mol×K	1103.93	Joback Method
cpg	1489.18	J/mol×K	1065.49	Joback Method
cpg	1551.18	J/mol×K	1257.68	Joback Method
dvisc	0.0000223	Pa×s	1027.05	Joback Method

dvisc	0.0000299	Pa×s	949.23	Joback Method
dvisc	0.0000423	Pa×s	871.42	Joback Method
dvisc	0.0000641	Pa×s	793.61	Joback Method
dvisc	0.0001061	Pa×s	715.79	Joback Method
dvisc	0.0001988	Pa×s	637.97	Joback Method
dvisc	0.0004435	Pa×s	560.16	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=U339732&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