1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl dodecyl ester

Inchi: InChI=1S/C27H48O4/c1-2-3-4-5-6-7-8-9-10-16-21-30-26(28)24-19-14-15-20-25(24)27(29

InchiKey: YSMQZWNXWWFLLW-UHFFFAOYSA-N

Formula: C27H48O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-250.19	kJ/mol	Joback Method
hf	-1001.91	kJ/mol	Joback Method
hfus	56.00	kJ/mol	Joback Method
hvap	94.56	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.380		Crippen Method
mcvol	384.450	ml/mol	McGowan Method
pc	895.87	kPa	Joback Method
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
tb	1004.17	K	Joback Method
tc	1229.43	K	Joback Method
tf	548.89	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1406.37	J/mol×K	1004.17	Joback Method
cpg	1425.33	J/mol×K	1041.71	Joback Method
cpg	1442.17	J/mol×K	1079.26	Joback Method
cpg	1456.95	J/mol×K	1116.80	Joback Method
cpg	1469.72	J/mol×K	1154.34	Joback Method
cpg	1480.55	J/mol×K	1191.89	Joback Method
cpg	1489.48	J/mol×K	1229.43	Joback Method
dvisc	0.0005055	Pa×s	548.89	Joback Method

dvisc	0.0002284	Pa×s	624.77	Joback Method
dvisc	0.0001226	Pa×s	700.65	Joback Method
dvisc	0.0000743	Pa×s	776.53	Joback Method
dvisc	0.0000492	Pa×s	852.41	Joback Method
dvisc	0.0000349	Pa×s	928.29	Joback Method
dvisc	0.0000260	Pa×s	1004.17	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=U339746&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