1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylcyclohexyl dodecyl ester

Inchi: InChI=1S/C28H50O4/c1-4-5-6-7-8-9-10-11-12-15-18-31-27(29)25-16-13-14-17-26(25)28

InchiKey: FZIPNDRDSBTSIJ-UHFFFAOYSA-N

Formula: C28H50O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-257.19	kJ/mol	Joback Method
hf	-1063.23	kJ/mol	Joback Method
hfus	60.73	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-8.20		Crippen Method
logp	7.625		Crippen Method
mcvol	398.540	ml/mol	McGowan Method
pc	814.93	kPa	Joback Method
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
tb	1017.71	K	Joback Method
tc	1246.07	K	Joback Method
tf	551.68	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1478.72	J/mol×K	1017.71	Joback Method
cpg	1497.73	J/mol×K	1055.77	Joback Method
cpg	1514.34	J/mol×K	1093.83	Joback Method
cpg	1528.60	J/mol×K	1131.89	Joback Method
cpg	1540.55	J/mol×K	1169.95	Joback Method
cpg	1550.22	J/mol×K	1208.01	Joback Method
cpg	1557.68	J/mol×K	1246.07	Joback Method
dvisc	0.0005758	Pa×s	551.68	Joback Method

dvisc	0.0002821	Pa×s	629.35	Joback Method
dvisc	0.0001617	Pa×s	707.02	Joback Method
dvisc	0.0001035	Pa×s	784.69	Joback Method
dvisc	0.0000718	Pa×s	862.37	Joback Method
dvisc	0.0000529	Pa×s	940.04	Joback Method
dvisc	0.0000408	Pa×s	1017.71	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=U339854&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