1,2-Cyclohexanedicarboxylic acid, 2,5-dimethylphenyl dodecyl ester

Inchi: InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-12-15-20-31-27(29)24-16-13-14-17-25(24)28

InchiKey: ODVZOVYJHMPYGG-UHFFFAOYSA-N

Formula: C28H44O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-173.07	kJ/mol	Joback Method
hf	-863.28	kJ/mol	Joback Method
hfus	60.02	kJ/mol	Joback Method
hvap	99.95	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.479		Crippen Method
mcvol	385.640	ml/mol	McGowan Method
pc	895.87	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	1044.14	K	Joback Method
tc	1278.45	K	Joback Method
tf	604.24	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1367.10	J/mol×K	1044.14	Joback Method
cpg	1383.48	J/mol×K	1083.19	Joback Method
cpg	1397.83	J/mol×K	1122.24	Joback Method
cpg	1410.18	J/mol×K	1161.30	Joback Method
cpg	1420.59	J/mol×K	1200.35	Joback Method
cpg	1429.13	J/mol×K	1239.40	Joback Method
cpg	1435.83	J/mol×K	1278.45	Joback Method
dvisc	0.0002732	Pa×s	604.24	Joback Method

dvisc	0.0001462	Pa×s	677.56	Joback Method
dvisc	0.0000884	Pa×s	750.87	Joback Method
dvisc	0.0000585	Pa×s	824.19	Joback Method
dvisc	0.0000414	Pa×s	897.51	Joback Method
dvisc	0.0000308	Pa×s	970.82	Joback Method
dvisc	0.0000240	Pa×s	1044.14	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=U339945&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