1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl pentadecyl ester

Inchi: InChI=1S/C31H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-21-34-30(32)28-19-16-17-20

InchiKey: ARWFZOWRCXHPFK-UHFFFAOYSA-N

Formula: C31H50O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 486.73

Physical Properties

Property code	Value	Unit	Source
gf	-147.81	kJ/mol	Joback Method
hf	-925.20	kJ/mol	Joback Method
hfus	67.79	kJ/mol	Joback Method
hvap	106.63	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	8.650		Crippen Method
mcvol	427.910	ml/mol	McGowan Method
pc	759.32	kPa	Joback Method
rinpol	3551.00		NIST Webbook
rinpol	3551.00		NIST Webbook
tb	1112.78	K	Joback Method
tc	1369.64	K	Joback Method
tf	638.05	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1556.06	J/mol×K	1112.78	Joback Method
cpg	1613.17	J/mol×K	1326.83	Joback Method
cpg	1606.36	J/mol×K	1284.02	Joback Method
cpg	1597.33	J/mol×K	1241.21	Joback Method
cpg	1586.00	J/mol×K	1198.40	Joback Method
cpg	1572.27	J/mol×K	1155.59	Joback Method
cpg	1617.85	J/mol×K	1369.64	Joback Method
dvisc	0.0000151	Pa×s	1112.78	Joback Method

dvisc	0.0000196	Pa×s	1033.66	Joback Method
dvisc	0.0000266	Pa×s	954.54	Joback Method
dvisc	0.0000380	Pa×s	875.41	Joback Method
dvisc	0.0000583	Pa×s	796.29	Joback Method
dvisc	0.0000983	Pa×s	717.17	Joback Method
dvisc	0.0001887	Pa×s	638.05	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=U339622&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