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

Inchi: InChI=1S/C26H46O4/c1-4-5-6-7-8-9-10-13-16-29-25(27)23-14-11-12-15-24(23)26(28)30
InchiKey: JAZXRZZXMKPHSH-UHFFFAOYSA-N
Formula: C26H46O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-274.03	kJ/mol	Joback Method
hf	-1021.95	kJ/mol	Joback Method
hfus	55.55	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.845		Crippen Method
mcvol	370.360	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	971.95	K	Joback Method
tc	1191.21	K	Joback Method
tf	529.14	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.70	J/mol×K	971.95	Joback Method
cpg	1370.20	J/mol×K	1008.49	Joback Method
cpg	1387.53	J/mol×K	1045.04	Joback Method
cpg	1402.73	J/mol×K	1081.58	Joback Method
cpg	1415.84	J/mol×K	1118.12	Joback Method
cpg	1426.87	J/mol×K	1154.67	Joback Method
cpg	1435.87	J/mol×K	1191.21	Joback Method
dvisc	0.0007204	Pa×s	529.14	Joback Method

dvisc	0.0003599	Pa×s	602.94	Joback Method
dvisc	0.0002091	Pa×s	676.74	Joback Method
dvisc	0.0001352	Pa×s	750.55	Joback Method
dvisc	0.0000945	Pa×s	824.35	Joback Method
dvisc	0.0000701	Pa×s	898.15	Joback Method
dvisc	0.0000544	Pa×s	971.95	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=U339852&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