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

Inchi: InChI=1S/C26H40O4/c1-4-5-6-7-8-9-10-13-16-29-25(27)23-14-11-12-15-24(23)26(28)30
InchiKey: LEZCGOSBLSEKGG-UHFFFAOYSA-N
Formula: C26H40O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-189.91	kJ/mol	Joback Method
hf	-822.00	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	95.50	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.699		Crippen Method
mcvol	357.460	ml/mol	McGowan Method
pc	1008.45	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	998.38	K	Joback Method
tc	1223.52	K	Joback Method
tf	581.70	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.11	J/mol×K	998.38	Joback Method
cpg	1258.67	J/mol×K	1035.90	Joback Method
cpg	1273.38	J/mol×K	1073.43	Joback Method
cpg	1286.27	J/mol×K	1110.95	Joback Method
cpg	1297.40	J/mol×K	1148.47	Joback Method
cpg	1306.80	J/mol×K	1186.00	Joback Method
cpg	1314.51	J/mol×K	1223.52	Joback Method
dvisc	0.0003449	Pa×s	581.70	Joback Method

dvisc	0.0001882	Pa×s	651.15	Joback Method
dvisc	0.0001155	Pa×s	720.59	Joback Method
dvisc	0.0000772	Pa×s	790.04	Joback Method
dvisc	0.0000550	Pa×s	859.49	Joback Method
dvisc	0.0000413	Pa×s	928.93	Joback Method
dvisc	0.0000323	Pa×s	998.38	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=U339619&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