1,2-Cyclohexanedicarboxylic acid, decyl 3-methylphenyl ester

Inchi: InChI=1S/C25H38O4/c1-3-4-5-6-7-8-9-12-18-28-24(26)22-16-10-11-17-23(22)25(27)29-2
InchiKey: JVSSVWTXKDONDH-UHFFFAOYSA-N
Formula: C25H38O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-188.70	kJ/mol	Joback Method
hf	-789.89	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.391		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
tb	970.52	K	Joback Method
tc	1191.66	K	Joback Method
tf	557.91	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.70	J/mol×K	970.52	Joback Method
cpg	1247.86	J/mol×K	1154.81	Joback Method
cpg	1237.75	J/mol×K	1117.95	Joback Method
cpg	1226.02	J/mol×K	1081.09	Joback Method
cpg	1212.63	J/mol×K	1044.23	Joback Method
cpg	1197.54	J/mol×K	1007.38	Joback Method
cpg	1256.40	J/mol×K	1191.66	Joback Method
dvisc	0.0000364	Pa×s	970.52	Joback Method

dvisc	0.0000471	Pa×s	901.75	Joback Method
dvisc	0.0000634	Pa×s	832.98	Joback Method
dvisc	0.0000902	Pa×s	764.21	Joback Method
dvisc	0.0001375	Pa×s	695.45	Joback Method
dvisc	0.0002300	Pa×s	626.68	Joback Method
dvisc	0.0004367	Pa×s	557.91	Joback Method

Sources

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=U339837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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