1,2-Cyclohexanedicarboxylic acid, dodecyl hexyl ester

Inchi: InChI=1S/C26H48O4/c1-3-5-7-9-10-11-12-13-14-18-22-30-26(28)24-20-16-15-19-23(24)25(27)29-21-17-8-6-4-2/h23-24H,3-22H2,1-2H3

InchiKey: BVVIURIMFIHNRV-UHFFFAOYSA-N

Formula: C26H48O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-283.06	kJ/mol	Joback Method
hf	-1035.59	kJ/mol	Joback Method
hfus	61.58	kJ/mol	Joback Method
hvap	91.90	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.380		Crippen Method
mcvol	381.220	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	961.74	K	Joback Method
tc	1178.14	K	Joback Method
tf	530.24	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.18	J/mol×K	961.74	Joback Method
cpg	1366.30	J/mol×K	997.81	Joback Method
cpg	1384.59	J/mol×K	1033.87	Joback Method
cpg	1401.10	J/mol×K	1069.94	Joback Method
cpg	1415.87	J/mol×K	1106.01	Joback Method
cpg	1428.94	J/mol×K	1142.08	Joback Method
cpg	1440.35	J/mol×K	1178.14	Joback Method
dvisc	0.0005127	Pa×s	530.24	Joback Method

dvisc	0.0002399	Pa×s	602.16	Joback Method
dvisc	0.0001320	Pa×s	674.07	Joback Method
dvisc	0.0000815	Pa×s	745.99	Joback Method
dvisc	0.0000548	Pa×s	817.91	Joback Method
dvisc	0.0000393	Pa×s	889.82	Joback Method
dvisc	0.0000296	Pa×s	961.74	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=U339417&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