1,2-Cyclohexanedicarboxylic acid, dodecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C26H48O4/c1-5-7-8-9-10-11-12-13-14-17-20-29-25(27)22-18-15-16-19-23(22)

InchiKey: QOKKJVWLZSKILP-UHFFFAOYSA-N

Formula: C26H48O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-287.94	kJ/mol	Joback Method
hf	-1046.15	kJ/mol	Joback Method
hfus	54.53	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.235		Crippen Method
mcvol	381.220	ml/mol	McGowan Method
pc	848.01	kPa	Joback Method
rinpol	2877.00		NIST Webbook
rinpol	2877.00		NIST Webbook
tb	960.86	K	Joback Method
tc	1176.44	K	Joback Method
tf	500.24	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.89	J/mol×K	960.86	Joback Method
cpg	1428.74	J/mol×K	1140.51	Joback Method
cpg	1415.87	J/mol×K	1104.58	Joback Method
cpg	1401.30	J/mol×K	1068.65	Joback Method
cpg	1384.97	J/mol×K	1032.72	Joback Method
cpg	1366.85	J/mol×K	996.79	Joback Method
cpg	1439.93	J/mol×K	1176.44	Joback Method
dvisc	0.0000245	Pa×s	960.86	Joback Method

dvisc	0.0000335	Pa×s	884.09	Joback Method
dvisc	0.0000486	Pa×s	807.32	Joback Method
dvisc	0.0000761	Pa×s	730.55	Joback Method
dvisc	0.0001324	Pa×s	653.78	Joback Method
dvisc	0.0002670	Pa×s	577.01	Joback Method
dvisc	0.0006680	Pa×s	500.24	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=U339449&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