cis-Cyclohex-4-en-1,2-dicarboxylic acid, dodecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C26H46O4/c1-5-7-8-9-10-11-12-13-14-17-20-29-25(27)22-18-15-16-19-23(22)26(28)30-24(21(4)6-2)3/h15-16,21-24H,5-14,17-20H2,1-4H3/t21-,22+,23-,24?/m0/s1

InchiKey: GYYQYKSPVQHJTI-UHFFFAOYSA-N

Formula: C26H46O4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-257.98	kJ/mol	Joback Method
hf	-988.37	kJ/mol	Joback Method
hfus	55.75	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.011		Crippen Method
mcvol	376.920	ml/mol	McGowan Method
pc	866.07	kPa	Joback Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook
tb	960.02	K	Joback Method
tc	1175.36	K	Joback Method
tf	501.00	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.86	J/mol×K	960.02	Joback Method
cpg	1335.16	J/mol×K	995.91	Joback Method
cpg	1352.69	J/mol×K	1031.80	Joback Method
cpg	1368.49	J/mol×K	1067.69	Joback Method
cpg	1382.61	J/mol×K	1103.58	Joback Method
cpg	1395.09	J/mol×K	1139.47	Joback Method
cpg	1405.97	J/mol×K	1175.36	Joback Method
dvisc	0.0006585	Pa×s	501.00	Joback Method

dvisc	0.0002714	Pa×s	577.50	Joback Method
dvisc	0.0001377	Pa×s	654.01	Joback Method
dvisc	0.0000805	Pa×s	730.51	Joback Method
dvisc	0.0000521	Pa×s	807.01	Joback Method
dvisc	0.0000364	Pa×s	883.52	Joback Method
dvisc	0.0000269	Pa×s	960.02	Joback Method

Sources

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=U382768&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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