1,2-Cyclohexanedicarboxylic acid, dodecyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C27H48O4/c1-3-4-5-6-7-8-9-10-11-16-21-30-26(28)23-18-13-14-19-24(23)27(2

InchiKey: XALYPGLCLYRQJH-UHFFFAOYSA-N

Formula: C27H48O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-257.90	kJ/mol	Joback Method
hf	-1022.25	kJ/mol	Joback Method
hfus	57.07	kJ/mol	Joback Method
hvap	94.25	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.379		Crippen Method
mcvol	384.450	ml/mol	McGowan Method
pc	878.44	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	999.50	K	Joback Method
tc	1223.76	K	Joback Method
tf	544.65	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.52	J/mol×K	999.50	Joback Method
cpg	1429.61	J/mol×K	1036.88	Joback Method
cpg	1446.51	J/mol×K	1074.25	Joback Method
cpg	1461.26	J/mol×K	1111.63	Joback Method
cpg	1473.90	J/mol×K	1149.01	Joback Method
cpg	1484.49	J/mol×K	1186.39	Joback Method
cpg	1493.07	J/mol×K	1223.76	Joback Method
dvisc	0.0005729	Pa×s	544.65	Joback Method

dvisc	0.0002706	Pa×s	620.46	Joback Method
dvisc	0.0001505	Pa×s	696.27	Joback Method
dvisc	0.0000940	Pa×s	772.08	Joback Method
dvisc	0.0000638	Pa×s	847.88	Joback Method
dvisc	0.0000462	Pa×s	923.69	Joback Method
dvisc	0.0000351	Pa×s	999.50	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=U339882&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