1,2-Cyclohexanedicarboxylic acid, allyl dodecyl ester

Inchi: InChI=1S/C23H40O4/c1-3-5-6-7-8-9-10-11-12-15-19-27-23(25)21-17-14-13-16-20(21)22

InchiKey: WIGNXGQJIPTUFK-UHFFFAOYSA-N

Formula: C23H40O4

SMILES: C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-220.48	kJ/mol	Joback Method
hf	-848.24	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	84.55	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.986		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	889.78	K	Joback Method
tc	1091.86	K	Joback Method
tf	494.67	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.94	J/mol×K	889.78	Joback Method
cpg	1146.08	J/mol×K	923.46	Joback Method
cpg	1163.76	J/mol×K	957.14	Joback Method
cpg	1180.00	J/mol×K	990.82	Joback Method
cpg	1194.84	J/mol×K	1024.50	Joback Method
cpg	1208.30	J/mol×K	1058.18	Joback Method
cpg	1220.42	J/mol×K	1091.86	Joback Method
dvisc	0.0007489	Pa×s	494.67	Joback Method

dvisc	0.0003652	Pa×s	560.52	Joback Method
dvisc	0.0002071	Pa×s	626.37	Joback Method
dvisc	0.0001308	Pa×s	692.23	Joback Method
dvisc	0.0000895	Pa×s	758.08	Joback Method
dvisc	0.0000651	Pa×s	823.93	Joback Method
dvisc	0.0000496	Pa×s	889.78	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=U339490&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