1,2-Cyclohexanedicarboxylic acid, allyl pentadecyl ester

Inchi: InChI=1S/C26H46O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-18-22-30-26(28)24-20-17-16-19

InchiKey: KPFHTFCFTOPOEV-UHFFFAOYSA-N

Formula: C26H46O4

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

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-195.22	kJ/mol	Joback Method
hf	-910.16	kJ/mol	Joback Method
hfus	60.30	kJ/mol	Joback Method
hvap	91.23	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.156		Crippen Method
mcvol	376.920	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	2961.00		NIST Webbook
rinpol	2961.00		NIST Webbook
tb	958.42	K	Joback Method
tc	1173.63	K	Joback Method
tf	528.48	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.34	J/mol×K	958.42	Joback Method
cpg	1335.99	J/mol×K	994.29	Joback Method
cpg	1353.90	J/mol×K	1030.16	Joback Method
cpg	1370.12	J/mol×K	1066.02	Joback Method
cpg	1384.69	J/mol×K	1101.89	Joback Method
cpg	1397.68	J/mol×K	1137.76	Joback Method
cpg	1409.11	J/mol×K	1173.63	Joback Method
dvisc	0.0005284	Pa×s	528.48	Joback Method

dvisc	0.0002503	Pa×s	600.14	Joback Method
dvisc	0.0001391	Pa×s	671.79	Joback Method
dvisc	0.0000865	Pa×s	743.45	Joback Method
dvisc	0.0000585	Pa×s	815.11	Joback Method
dvisc	0.0000422	Pa×s	886.76	Joback Method
dvisc	0.0000319	Pa×s	958.42	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=U339492&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