1,2-Cyclohexanedicarboxylic acid, allyl hexadecyl ester

Inchi: InChI=1S/C27H48O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-23-31-27(29)25-21-18-17

InchiKey: MXBJKTJQZPZNOD-UHFFFAOYSA-N

Formula: C27H48O4

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

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-186.80	kJ/mol	Joback Method
hf	-930.80	kJ/mol	Joback Method
hfus	62.89	kJ/mol	Joback Method
hvap	93.46	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.546		Crippen Method
mcvol	391.010	ml/mol	McGowan Method
pc	814.46	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	981.30	K	Joback Method
tc	1202.91	K	Joback Method
tf	539.75	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.25	J/mol×K	981.30	Joback Method
cpg	1400.12	J/mol×K	1018.24	Joback Method
cpg	1418.13	J/mol×K	1055.17	Joback Method
cpg	1434.34	J/mol×K	1092.11	Joback Method
cpg	1448.80	J/mol×K	1129.04	Joback Method
cpg	1461.56	J/mol×K	1165.98	Joback Method
cpg	1472.69	J/mol×K	1202.91	Joback Method
dvisc	0.0004674	Pa×s	539.75	Joback Method

dvisc	0.0002195	Pa×s	613.34	Joback Method
dvisc	0.0001212	Pa×s	686.93	Joback Method
dvisc	0.0000751	Pa×s	760.53	Joback Method
dvisc	0.0000506	Pa×s	834.12	Joback Method
dvisc	0.0000364	Pa×s	907.71	Joback Method
dvisc	0.0000274	Pa×s	981.30	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=U339493&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

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