1,2-Cyclohexanedicarboxylic acid, allyl propyl ester

Inchi: InChI=1S/C14H22O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3,11-12H,1,4-

InchiKey: NRNACEABKBLQSA-UHFFFAOYSA-N

Formula: C14H22O4

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

Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-296.26	kJ/mol	Joback Method
hf	-662.48	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.475		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	683.86	K	Joback Method
tc	886.72	K	Joback Method
tf	393.24	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.40	J/mol×K	683.86	Joback Method
cpg	672.92	J/mol×K	852.91	Joback Method
cpg	659.34	J/mol×K	819.10	Joback Method
cpg	644.70	J/mol×K	785.29	Joback Method
cpg	629.01	J/mol×K	751.48	Joback Method
cpg	612.24	J/mol×K	717.67	Joback Method
cpg	685.45	J/mol×K	886.72	Joback Method
dvisc	0.0001601	Pa×s	683.86	Joback Method

dvisc	0.0002041	Pa×s	635.42	Joback Method
dvisc	0.0002708	Pa×s	586.99	Joback Method
dvisc	0.0003780	Pa×s	538.55	Joback Method
dvisc	0.0005636	Pa×s	490.11	Joback Method
dvisc	0.0009172	Pa×s	441.68	Joback Method
dvisc	0.0016830	Pa×s	393.24	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=U339479&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