1,2-Cyclohexanedicarboxylic acid, allyl isohexyl ester

Inchi: InChI=1S/C17H28O4/c1-4-11-20-16(18)14-9-5-6-10-15(14)17(19)21-12-7-8-13(2)3/h4,13

InchiKey: LWLZLLLXKPWEIQ-UHFFFAOYSA-N

Formula: C17H28O4

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

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-273.44	kJ/mol	Joback Method
hf	-729.68	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.501		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	752.06	K	Joback Method
tc	952.12	K	Joback Method
tf	412.05	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.52	J/mol×K	752.06	Joback Method
cpg	783.24	J/mol×K	785.40	Joback Method
cpg	800.75	J/mol×K	818.75	Joback Method
cpg	817.04	J/mol×K	852.09	Joback Method
cpg	832.15	J/mol×K	885.43	Joback Method
cpg	846.08	J/mol×K	918.78	Joback Method
cpg	858.85	J/mol×K	952.12	Joback Method
dvisc	0.0015957	Pa×s	412.05	Joback Method

dvisc	0.0007670	Pa×s	468.72	Joback Method
dvisc	0.0004318	Pa×s	525.39	Joback Method
dvisc	0.0002718	Pa×s	582.05	Joback Method
dvisc	0.0001858	Pa×s	638.72	Joback Method
dvisc	0.0001351	Pa×s	695.39	Joback Method
dvisc	0.0001031	Pa×s	752.06	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=U339483&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