1,2-Cyclohexanedicarboxylic acid, allyl isobutyl ester

Inchi: InChI=1S/C15H24O4/c1-4-9-18-14(16)12-7-5-6-8-13(12)15(17)19-10-11(2)3/h4,11-13H,1

InchiKey: VEXMRTBLPHFSDY-UHFFFAOYSA-N

Formula: C15H24O4

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

Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-290.28	kJ/mol	Joback Method
hf	-688.40	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	66.36	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.721		Crippen Method
mcvol	221.930	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	706.30	K	Joback Method
tc	910.13	K	Joback Method
tf	389.51	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.33	J/mol×K	706.30	Joback Method
cpg	668.74	J/mol×K	740.27	Joback Method
cpg	686.00	J/mol×K	774.24	Joback Method
cpg	702.11	J/mol×K	808.22	Joback Method
cpg	717.08	J/mol×K	842.19	Joback Method
cpg	730.93	J/mol×K	876.16	Joback Method
cpg	743.66	J/mol×K	910.13	Joback Method
dvisc	0.0018834	Pa×s	389.51	Joback Method

dvisc	0.0009283	Pa×s	442.31	Joback Method
dvisc	0.0005320	Pa×s	495.11	Joback Method
dvisc	0.0003395	Pa×s	547.90	Joback Method
dvisc	0.0002344	Pa×s	600.70	Joback Method
dvisc	0.0001718	Pa×s	653.50	Joback Method
dvisc	0.0001320	Pa×s	706.30	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=U339480&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