1,2-Cyclohexanedicarboxylic acid, ethyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C15H26O4/c1-5-18-14(16)12-8-6-7-9-13(12)15(17)19-11(4)10(2)3/h10-13H,5-9

InchiKey: ZAWZBUBPCGLSPK-UHFFFAOYSA-N

Formula: C15H26O4

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

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-380.56	kJ/mol	Joback Method
hf	-819.11	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.944		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1746.00		NIST Webbook
tb	709.18	K	Joback Method
tc	913.13	K	Joback Method
tf	376.27	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.17	J/mol×K	709.18	Joback Method
cpg	694.38	J/mol×K	743.17	Joback Method
cpg	712.39	J/mol×K	777.16	Joback Method
cpg	729.21	J/mol×K	811.16	Joback Method
cpg	744.83	J/mol×K	845.15	Joback Method
cpg	759.27	J/mol×K	879.14	Joback Method
cpg	772.52	J/mol×K	913.13	Joback Method
dvisc	0.0023439	Pa×s	376.27	Joback Method
dvisc	0.0010286	Pa×s	431.75	Joback Method

dvisc	0.0005445	Pa×s	487.24	Joback Method
dvisc	0.0003283	Pa×s	542.72	Joback Method
dvisc	0.0002174	Pa×s	598.21	Joback Method
dvisc	0.0001544	Pa×s	653.69	Joback Method
dvisc	0.0001157	Pa×s	709.18	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=U339557&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