Cyclohexanecarboxylic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C12H22O2/c1-9(2)10(3)14-12(13)11-7-5-4-6-8-11/h9-11H,4-8H2,1-3H3
InchiKey: VJIWTPJDGKMXCO-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CC(C)C(C)OC(=O)C1CCCCC1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-164.19	kJ/mol	Joback Method
hf	-492.05	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.154		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1361.00		NIST Webbook
tb	568.92	K	Joback Method
tc	776.71	K	Joback Method
tf	274.54	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.09	J/mol×K	568.92	Joback Method
cpg	475.09	J/mol×K	603.55	Joback Method
cpg	494.01	J/mol×K	638.18	Joback Method
cpg	511.87	J/mol×K	672.82	Joback Method
cpg	528.70	J/mol×K	707.45	Joback Method
cpg	544.51	J/mol×K	742.08	Joback Method
cpg	559.32	J/mol×K	776.71	Joback Method
dvisc	0.0077961	Pa×s	274.54	Joback Method
dvisc	0.0025713	Pa×s	323.60	Joback Method

dvisc	0.0011357	Pa×s	372.67	Joback Method
dvisc	0.0006067	Pa×s	421.73	Joback Method
dvisc	0.0003693	Pa×s	470.79	Joback Method
dvisc	0.0002469	Pa×s	519.86	Joback Method
dvisc	0.0001769	Pa×s	568.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354646&Units=SI
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

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