Cyclohexanecarboxylic acid, heptyl ester

Other names: heptyl cyclohexanecarboxylate
Inchi: InChI=1S/C14H26O2/c1-2-3-4-5-9-12-16-14(15)13-10-7-6-8-11-13/h13H,2-12H2,1H3
InchiKey: NUUQQOTYKFJRDX-UHFFFAOYSA-N
Formula: C14H26O2
SMILES: CCCCCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 226.35
CAS: 92319-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-142.47	kJ/mol	Joback Method
hf	-522.77	kJ/mol	Joback Method
hfus	26.64	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.080		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1606.09		NIST Webbook
rinpol	1609.01		NIST Webbook
rinpol	1606.09		NIST Webbook
tb	615.56	K	Joback Method
tc	809.77	K	Joback Method
tf	327.08	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.97	J/mol×K	615.56	Joback Method
cpg	579.88	J/mol×K	647.93	Joback Method
cpg	598.76	J/mol×K	680.30	Joback Method
cpg	616.63	J/mol×K	712.67	Joback Method
cpg	633.51	J/mol×K	745.04	Joback Method

cpg	649.42	J/mol×K	777.41	Joback Method
cpg	664.38	J/mol×K	809.77	Joback Method
dvisc	0.0034050	Pa×s	327.08	Joback Method
dvisc	0.0014830	Pa×s	375.16	Joback Method
dvisc	0.0007802	Pa×s	423.24	Joback Method
dvisc	0.0004679	Pa×s	471.32	Joback Method
dvisc	0.0003085	Pa×s	519.40	Joback Method
dvisc	0.0002182	Pa×s	567.48	Joback Method
dvisc	0.0001630	Pa×s	615.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92319476&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