Cyclohexyl nonanoate

Other names: Cyclohexyl nonanoate
Nonoic acid, cyclohexyl ester
Inchi: InChI=1S/C15H28O2/c1-2-3-4-5-6-10-13-15(16)17-14-11-8-7-9-12-14/h14H,2-13H2,1H3
InchiKey: ZXGCFXPVWOGXMA-UHFFFAOYSA-N
Formula: C15H28O2
SMILES: CCCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]: 240.39

Physical Properties

Property code	Value	Unit	Source
af	0.6979		Cheméo Relay (1.0)
hf	-636.07	kJ/mol	Cheméo Relay (1.0)
hfus	29.23	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-4.92		Cheméo Relay (1.0)
logp	4.613		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1736.00		NIST Webbook
rinpol	1702.00		NIST Webbook
tb	562.81	K	Cheméo Relay (1.0)
tc	768.80	K	Cheméo Relay (1.0)
tf	256.16	K	Cheméo Relay (1.0)
vc	0.823	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.82	J/mol×K	638.44	Joback Method
cpg	720.72	J/mol×K	830.44	Joback Method
cpg	705.57	J/mol×K	798.44	Joback Method
cpg	689.44	J/mol×K	766.44	Joback Method
cpg	672.33	J/mol×K	734.44	Joback Method

cpg	654.20	J/mol×K	702.44	Joback Method
cpg	635.04	J/mol×K	670.44	Joback Method
dvisc	0.0004219	Pa×s	488.39	Joback Method
dvisc	0.0001453	Pa×s	638.44	Joback Method
dvisc	0.0001951	Pa×s	588.42	Joback Method
dvisc	0.0002768	Pa×s	538.41	Joback Method
dvisc	0.0031539	Pa×s	338.35	Joback Method
dvisc	0.0007079	Pa×s	438.38	Joback Method
dvisc	0.0013572	Pa×s	388.37	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358024&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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