cyclohexanecarboxylic acid, nonyl ester

Other names: nonyl cyclohexanecarboxylate
Inchi: InChI=1S/C16H30O2/c1-2-3-4-5-6-7-11-14-18-16(17)15-12-9-8-10-13-15/h15H,2-14H2,1
InchiKey: VRJLOADUMBZEBS-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CCCCCCCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
af	0.7169		Cheméo Relay (1.0)
hf	-630.78	kJ/mol	Cheméo Relay (1.0)
hfus	31.82	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.29		Cheméo Relay (1.0)
logp	4.861		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1808.99		NIST Webbook
rinpol	1806.51		NIST Webbook
rinpol	1806.51		NIST Webbook
tb	583.48	K	Cheméo Relay (1.0)
tc	785.49	K	Cheméo Relay (1.0)
tf	277.67	K	Cheméo Relay (1.0)
vc	0.869	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.95	J/mol×K	661.32	Joback Method
cpg	691.42	J/mol×K	693.00	Joback Method
cpg	710.81	J/mol×K	724.69	Joback Method
cpg	729.14	J/mol×K	756.37	Joback Method
cpg	746.44	J/mol×K	788.05	Joback Method
cpg	762.73	J/mol×K	819.74	Joback Method

cpg	778.03	J/mol×K	851.42	Joback Method
dvisc	0.0028997	Pa×s	349.62	Joback Method
dvisc	0.0012337	Pa×s	401.57	Joback Method
dvisc	0.0006384	Pa×s	453.52	Joback Method
dvisc	0.0003783	Pa×s	505.47	Joback Method
dvisc	0.0002471	Pa×s	557.42	Joback Method
dvisc	0.0001736	Pa×s	609.37	Joback Method
dvisc	0.0001289	Pa×s	661.32	Joback Method

Sources

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=C70289371&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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

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