Nonoic acid, cyclohexylmethyl ester

Other names: Nonoic acid, cyclohexylmethyl ester
Inchi: InChI=1S/C16H30O2/c1-2-3-4-5-6-10-13-16(17)18-14-15-11-8-7-9-12-15/h15H,2-14H2,1
InchiKey: CDDROYYAMGWVDA-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CCCCCCCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
af	0.7156		Cheméo Relay (1.0)
gf	-125.63	kJ/mol	Joback Method
hf	-654.15	kJ/mol	Cheméo Relay (1.0)
hfus	31.82	kJ/mol	Joback Method
hvap	77.11	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-5.20		Cheméo Relay (1.0)
logp	4.861		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	591.23	K	Cheméo Relay (1.0)
tc	778.69	K	Cheméo Relay (1.0)
tf	248.51	K	Cheméo Relay (1.0)
vc	0.865	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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358025&Units=SI

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):

Legend

af: Acentric Factor
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
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