

Nonanoic 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:	CDDROYAMGWVDA-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CCCCCCCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
gf	-125.63	kJ/mol	Joback Method
hf	-564.05	kJ/mol	Joback Method
hfus	31.82	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.861		Crippen Method
mvol	232.880	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	661.32	K	Joback Method
tc	851.42	K	Joback Method
tf	349.62	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.95	J/molxK	661.32	Joback Method
cpg	691.42	J/molxK	693.00	Joback Method
cpg	710.81	J/molxK	724.69	Joback Method
cpg	729.14	J/molxK	756.37	Joback Method
cpg	746.44	J/molxK	788.05	Joback Method
cpg	762.73	J/molxK	819.74	Joback Method
cpg	778.03	J/molxK	851.42	Joback Method

dvisc	0.0028997	Paxs	349.62	Joback Method
dvisc	0.0012337	Paxs	401.57	Joback Method
dvisc	0.0006384	Paxs	453.52	Joback Method
dvisc	0.0003783	Paxs	505.47	Joback Method
dvisc	0.0002471	Paxs	557.42	Joback Method
dvisc	0.0001736	Paxs	609.37	Joback Method
dvisc	0.0001289	Paxs	661.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358025&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

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