

nonyl benzoate

Other names:	Benzoic acid, nonyl ester
Inchi:	InChI=1S/C16H24O2/c1-2-3-4-5-6-7-11-14-18-16(17)15-12-9-8-10-13-15/h8-10,12-13H,2
InchiKey:	VUHMHACHBVTPMF-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	248.36
CAS:	5451-95-6

Physical Properties

Property code	Value	Unit	Source
gf	-37.67	kJ/mol	Joback Method
hf	-381.84	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.594		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1885.24		NIST Webbook
rinpol	1909.71		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1859.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2357.00		NIST Webbook
ripol	2387.00		NIST Webbook
ripol	2366.00		NIST Webbook

ripol	2385.00		NIST Webbook
ripol	2374.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2406.00		NIST Webbook
tb	668.45	K	Joback Method
tc	863.72	K	Joback Method
tf	368.66	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.99	J/molxK	668.45	Joback Method
cpg	676.54	J/molxK	831.18	Joback Method
cpg	663.03	J/molxK	798.63	Joback Method
cpg	648.65	J/molxK	766.09	Joback Method
cpg	633.37	J/molxK	733.54	Joback Method
cpg	617.16	J/molxK	701.00	Joback Method
cpg	689.21	J/molxK	863.72	Joback Method
dvisc	0.0001218	Paxs	668.45	Joback Method
dvisc	0.0001593	Paxs	618.48	Joback Method
dvisc	0.0002183	Paxs	568.52	Joback Method
dvisc	0.0003180	Paxs	518.55	Joback Method
dvisc	0.0005018	Paxs	468.59	Joback Method
dvisc	0.0008831	Paxs	418.62	Joback Method
dvisc	0.0018111	Paxs	368.66	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451956&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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