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	1859.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1856.00		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	1870.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1885.24		NIST Webbook
rinpol	1909.71		NIST Webbook
rinpol	1857.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2375.00		NIST Webbook

ripol	2357.00		NIST Webbook
ripol	2387.00		NIST Webbook
ripol	2366.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2385.00		NIST Webbook
ripol	2374.00		NIST Webbook
tb	668.45	K	Joback Method
tc	863.72	K	Joback Method
tf	368.66	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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