Nonanoic acid, phenylmethyl ester

Other names:	Benzyl n-nonanoate
	Benzyl nonanoate
	benzyl nonan-1-oate
Inchi:	InChI=1S/C16H24O2/c1-2-3-4-5-6-10-13-16(17)18-14-15-11-8-7-9-12-15/h7-9,11-12H,2-
InchiKey:	KVIQEJMWUXBBQJ-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	248.36
CAS:	6471-66-5

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	-4.98		Crippen Method
logp	4.480		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
ripol	2362.00		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	617.16	J/mol×K	701.00	Joback Method

cpg	633.37	J/mol×K	733.54	Joback Method
cpg	648.65	J/mol×K	766.09	Joback Method
cpg	663.03	J/mol×K	798.63	Joback Method
cpg	676.54	J/mol×K	831.18	Joback Method
cpg	689.21	J/mol×K	863.72	Joback Method
dvisc	0.0018111	Pa×s	368.66	Joback Method
dvisc	0.0008831	Pa×s	418.62	Joback Method
dvisc	0.0005018	Pa×s	468.59	Joback Method
dvisc	0.0003180	Pa×s	518.55	Joback Method
dvisc	0.0002183	Pa×s	568.52	Joback Method
dvisc	0.0001593	Pa×s	618.48	Joback Method
dvisc	0.0001218	Pa×s	668.45	Joback Method

Sources

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=C6471665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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