Behenyl benzoate

Inchi: InChI=1S/C29H50O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-27-31-29
InchiKey: IACXYDVFQDGXJF-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 430.71
CAS: 103403-38-9

Physical Properties

Property code	Value	Unit	Source
gf	71.79	kJ/mol	Joback Method
hf	-650.16	kJ/mol	Joback Method
hfus	67.69	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-10.50		Crippen Method
logp	9.665		Crippen Method
mcvol	403.150	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	3264.00		NIST Webbook
rinpol	3264.00		NIST Webbook
tb	965.89	K	Joback Method
tc	1184.68	K	Joback Method
tf	515.17	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.52	J/mol×K	965.89	Joback Method
cpg	1405.79	J/mol×K	1002.36	Joback Method
cpg	1425.55	J/mol×K	1038.82	Joback Method
cpg	1443.89	J/mol×K	1075.29	Joback Method
cpg	1460.89	J/mol×K	1111.75	Joback Method
cpg	1476.64	J/mol×K	1148.22	Joback Method
cpg	1491.24	J/mol×K	1184.68	Joback Method

dvisc	0.0004593	Pa×s	515.17	Joback Method
dvisc	0.0001962	Pa×s	590.29	Joback Method
dvisc	0.0001016	Pa×s	665.41	Joback Method
dvisc	0.0000601	Pa×s	740.53	Joback Method
dvisc	0.0000392	Pa×s	815.65	Joback Method
dvisc	0.0000274	Pa×s	890.77	Joback Method
dvisc	0.0000203	Pa×s	965.89	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=C103403389&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume