4-butylbenzoic acid, nonyl ester

Inchi: InChI=1S/C20H32O2/c1-3-5-7-8-9-10-11-17-22-20(21)19-15-13-18(14-16-19)12-6-4-2/h1
InchiKey: XKLMVDBBEMBEFD-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
af	0.9361		Cheméo Relay (1.0)
gf	-13.62	kJ/mol	Joback Method
hf	-542.53	kJ/mol	Cheméo Relay (1.0)
hfus	43.99	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-6.62		Cheméo Relay (1.0)
logp	5.937		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2266.50		NIST Webbook
rinpol	2266.50		NIST Webbook
tb	627.18	K	Cheméo Relay (1.0)
tc	818.29	K	Cheméo Relay (1.0)
tf	270.64	K	Cheméo Relay (1.0)
vc	1.051	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.03	J/mol×K	764.95	Joback Method
cpg	844.22	J/mol×K	796.85	Joback Method
cpg	861.37	J/mol×K	828.75	Joback Method
cpg	877.51	J/mol×K	860.66	Joback Method
cpg	892.69	J/mol×K	892.56	Joback Method
cpg	906.93	J/mol×K	924.46	Joback Method

cpg	920.27	J/mol×K	956.36	Joback Method
dvisc	0.0010468	Pa×s	426.26	Joback Method
dvisc	0.0005209	Pa×s	482.71	Joback Method
dvisc	0.0003000	Pa×s	539.16	Joback Method
dvisc	0.0001918	Pa×s	595.61	Joback Method
dvisc	0.0001325	Pa×s	652.05	Joback Method
dvisc	0.0000971	Pa×s	708.50	Joback Method
dvisc	0.0000745	Pa×s	764.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292206&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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