

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
gf	-13.62	kJ/mol	Joback Method
hf	-475.87	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	72.21	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.937		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinsol	2266.50		NIST Webbook
tb	764.95	K	Joback Method
tc	956.36	K	Joback Method
tf	426.26	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.03	J/molxK	764.95	Joback Method
cpg	844.22	J/molxK	796.85	Joback Method
cpg	861.37	J/molxK	828.75	Joback Method
cpg	877.51	J/molxK	860.66	Joback Method
cpg	892.69	J/molxK	892.56	Joback Method
cpg	906.93	J/molxK	924.46	Joback Method
cpg	920.27	J/molxK	956.36	Joback Method
dvisc	0.0010468	Paxs	426.26	Joback Method
dvisc	0.0005209	Paxs	482.71	Joback Method

dvisc	0.0003000	Paxs	539.16	Joback Method
dvisc	0.0001918	Paxs	595.61	Joback Method
dvisc	0.0001325	Paxs	652.05	Joback Method
dvisc	0.0000971	Paxs	708.50	Joback Method
dvisc	0.0000745	Paxs	764.95	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=U292206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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