4-Butylbenzoic acid, octyl ester

Inchi: InChI=1S/C19H30O2/c1-3-5-7-8-9-10-16-21-19(20)18-14-12-17(13-15-18)11-6-4-2/h12-1
InchiKey: WOHCEFXPFWWXKJ-UHFFFAOYSA-N
Formula: C19H30O2
SMILES: CCCCCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 290.44
CAS: 128434-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-22.04	kJ/mol	Joback Method
hf	-455.23	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.546		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	742.07	K	Joback Method
tc	933.92	K	Joback Method
tf	414.99	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.84	J/mol×K	742.07	Joback Method
cpg	785.77	J/mol×K	774.05	Joback Method
cpg	802.70	J/mol×K	806.02	Joback Method
cpg	818.64	J/mol×K	838.00	Joback Method
cpg	833.64	J/mol×K	869.97	Joback Method
cpg	847.73	J/mol×K	901.95	Joback Method
cpg	860.92	J/mol×K	933.92	Joback Method

dvisc	0.0011420	Pa×s	414.99	Joback Method
dvisc	0.0005754	Pa×s	469.50	Joback Method
dvisc	0.0003344	Pa×s	524.02	Joback Method
dvisc	0.0002152	Pa×s	578.53	Joback Method
dvisc	0.0001495	Pa×s	633.04	Joback Method
dvisc	0.0001100	Pa×s	687.56	Joback Method
dvisc	0.0000846	Pa×s	742.07	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=C128434877&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