4-Butylbenzoic acid, octadecyl ester

Inchi: InChI=1S/C29H50O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-26-31-29(30)28-2
InchiKey: PKAPDTSUVWQODK-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 430.71

Physical Properties

Property code	Value	Unit	Source
gf	62.16	kJ/mol	Joback Method
hf	-661.63	kJ/mol	Joback Method
hfus	67.30	kJ/mol	Joback Method
hvap	92.24	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	9.447		Crippen Method
mcvol	403.150	ml/mol	McGowan Method
pc	754.74	kPa	Joback Method
rinpol	3232.90		NIST Webbook
rinpol	3232.90		NIST Webbook
tb	970.87	K	Joback Method
tc	1190.94	K	Joback Method
tf	527.69	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.47	J/mol×K	970.87	Joback Method
cpg	1475.81	J/mol×K	1154.26	Joback Method
cpg	1460.29	J/mol×K	1117.58	Joback Method
cpg	1443.48	J/mol×K	1080.90	Joback Method
cpg	1425.29	J/mol×K	1044.23	Joback Method
cpg	1405.65	J/mol×K	1007.55	Joback Method
cpg	1490.12	J/mol×K	1190.94	Joback Method
dvisc	0.0000208	Pa×s	970.87	Joback Method

dvisc	0.0000277	Pa×s	897.01	Joback Method
dvisc	0.0000389	Pa×s	823.14	Joback Method
dvisc	0.0000584	Pa×s	749.28	Joback Method
dvisc	0.0000958	Pa×s	675.42	Joback Method
dvisc	0.0001775	Pa×s	601.55	Joback Method
dvisc	0.0003908	Pa×s	527.69	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=U292330&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