4-Butylbenzoic acid, 3-pentadecyl ester

Inchi: InChI=1S/C26H44O2/c1-4-7-9-10-11-12-13-14-15-16-18-25(6-3)28-26(27)24-21-19-23(2
InchiKey: AVNOFVVLPCGKLL-UHFFFAOYSA-N
Formula: C26H44O2
SMILES: CCCCCCCCCCCCCC(CC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 388.63

Physical Properties

Property code	Value	Unit	Source
gf	34.46	kJ/mol	Joback Method
hf	-604.99	kJ/mol	Joback Method
hfus	56.01	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	8.276		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	894.27	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	901.79	K	Joback Method
tc	1104.83	K	Joback Method
tf	478.88	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.09	J/mol×K	901.79	Joback Method
cpg	1212.95	J/mol×K	935.63	Joback Method
cpg	1231.52	J/mol×K	969.47	Joback Method
cpg	1248.82	J/mol×K	1003.31	Joback Method
cpg	1264.94	J/mol×K	1037.15	Joback Method
cpg	1279.91	J/mol×K	1070.99	Joback Method
cpg	1293.79	J/mol×K	1104.83	Joback Method
dvisc	0.0006471	Pa×s	478.88	Joback Method

dvisc	0.0002785	Pa×s	549.37	Joback Method
dvisc	0.0001452	Pa×s	619.85	Joback Method
dvisc	0.0000865	Pa×s	690.34	Joback Method
dvisc	0.0000567	Pa×s	760.82	Joback Method
dvisc	0.0000399	Pa×s	831.31	Joback Method
dvisc	0.0000297	Pa×s	901.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299944&Units=SI

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