4-Butylbenzoic acid, heptadecyl ester

Inchi: InChI=1S/C28H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-25-30-28(29)27-23-2
InchiKey: VRWCPSOWOJJUQU-UHFFFAOYSA-N
Formula: C28H48O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	53.74	kJ/mol	Joback Method
hf	-640.99	kJ/mol	Joback Method
hfus	64.71	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	9.057		Crippen Method
mcvol	389.060	ml/mol	McGowan Method
pc	796.18	kPa	Joback Method
rinpol	2892.70		NIST Webbook
tb	947.99	K	Joback Method
tc	1161.23	K	Joback Method
tf	516.42	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.05	J/mol×K	947.99	Joback Method
cpg	1340.74	J/mol×K	983.53	Joback Method
cpg	1359.98	J/mol×K	1019.07	Joback Method
cpg	1377.85	J/mol×K	1054.61	Joback Method
cpg	1394.42	J/mol×K	1090.15	Joback Method
cpg	1409.76	J/mol×K	1125.69	Joback Method
cpg	1423.94	J/mol×K	1161.23	Joback Method
dvisc	0.0004423	Pa×s	516.42	Joback Method
dvisc	0.0002026	Pa×s	588.35	Joback Method

dvisc	0.0001100	Pa×s	660.28	Joback Method
dvisc	0.0000674	Pa×s	732.20	Joback Method
dvisc	0.0000450	Pa×s	804.13	Joback Method
dvisc	0.0000322	Pa×s	876.06	Joback Method
dvisc	0.0000242	Pa×s	947.99	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=U292213&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