4-Butylbenzoic acid, 3-tetradecyl ester

Inchi: InChI=1S/C25H42O2/c1-4-7-9-10-11-12-13-14-15-17-24(6-3)27-25(26)23-20-18-22(19-2
InchiKey: ODCXTOCTWDASFI-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
gf	26.04	kJ/mol	Joback Method
hf	-584.35	kJ/mol	Joback Method
hfus	53.42	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	7.886		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	947.91	kPa	Joback Method
rinpol	2629.00		NIST Webbook
tb	878.91	K	Joback Method
tc	1078.47	K	Joback Method
tf	467.61	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.24	J/mol×K	878.91	Joback Method
cpg	1149.81	J/mol×K	912.17	Joback Method
cpg	1168.12	J/mol×K	945.43	Joback Method
cpg	1185.24	J/mol×K	978.69	Joback Method
cpg	1201.20	J/mol×K	1011.95	Joback Method
cpg	1216.06	J/mol×K	1045.21	Joback Method
cpg	1229.87	J/mol×K	1078.47	Joback Method
dvisc	0.0007290	Pa×s	467.61	Joback Method
dvisc	0.0003164	Pa×s	536.16	Joback Method

dvisc	0.0001659	Pa×s	604.71	Joback Method
dvisc	0.0000992	Pa×s	673.26	Joback Method
dvisc	0.0000653	Pa×s	741.81	Joback Method
dvisc	0.0000461	Pa×s	810.36	Joback Method
dvisc	0.0000344	Pa×s	878.91	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=U299941&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