4-Butylbenzoic acid, 3-tridecyl ester

Inchi: InChI=1S/C24H40O2/c1-4-7-9-10-11-12-13-14-16-23(6-3)26-24(25)22-19-17-21(18-20-2
InchiKey: JHUAEUJUFMGOHU-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: CCCCCCCCCCC(CC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 360.57

Physical Properties

Property code	Value	Unit	Source
gf	17.62	kJ/mol	Joback Method
hf	-563.71	kJ/mol	Joback Method
hfus	50.83	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.495		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	856.03	K	Joback Method
tc	1052.96	K	Joback Method
tf	456.34	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.02	J/mol×K	856.03	Joback Method
cpg	1087.32	J/mol×K	888.85	Joback Method
cpg	1105.41	J/mol×K	921.67	Joback Method
cpg	1122.35	J/mol×K	954.50	Joback Method
cpg	1138.18	J/mol×K	987.32	Joback Method
cpg	1152.93	J/mol×K	1020.14	Joback Method
cpg	1166.67	J/mol×K	1052.96	Joback Method
dvisc	0.0008185	Pa×s	456.34	Joback Method
dvisc	0.0003584	Pa×s	522.95	Joback Method

dvisc	0.0001891	Pa×s	589.57	Joback Method
dvisc	0.0001136	Pa×s	656.18	Joback Method
dvisc	0.0000750	Pa×s	722.80	Joback Method
dvisc	0.0000531	Pa×s	789.41	Joback Method
dvisc	0.0000397	Pa×s	856.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299937&Units=SI
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

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