

Benzoic acid, 4-tert-butyl-, dodecyl ester

Inchi:	InChI=1S/C23H38O2/c1-5-6-7-8-9-10-11-12-13-14-19-25-22(24)20-15-17-21(18-16-20)2
InchiKey:	RHDFUFGFLNMALK-UHFFFAOYSA-N
Formula:	C23H38O2
SMILES:	CCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	346.55

Physical Properties

Property code	Value	Unit	Source
gf	14.48	kJ/mol	Joback Method
hf	-546.54	kJ/mol	Joback Method
hfus	44.35	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	7.062		Crippen Method
mvol	318.610	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	830.36	K	Joback Method
tc	1028.02	K	Joback Method
tf	462.49	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.77	J/molxK	830.36	Joback Method
cpg	1025.85	J/molxK	863.30	Joback Method
cpg	1043.77	J/molxK	896.25	Joback Method
cpg	1060.60	J/molxK	929.19	Joback Method
cpg	1076.40	J/molxK	962.14	Joback Method
cpg	1091.21	J/molxK	995.08	Joback Method
cpg	1105.10	J/molxK	1028.02	Joback Method
dvisc	0.0007464	Paxs	462.49	Joback Method

dvisc	0.0003434	Paxs	523.80	Joback Method
dvisc	0.0001859	Paxs	585.11	Joback Method
dvisc	0.0001131	Paxs	646.42	Joback Method
dvisc	0.0000750	Paxs	707.74	Joback Method
dvisc	0.0000531	Paxs	769.05	Joback Method
dvisc	0.0000395	Paxs	830.36	Joback Method

Sources

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=U406148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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