4-Butylbenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C21H28O2/c1-6-7-8-18-10-12-19(13-11-18)21(22)23-20(15-17(4)5)14-9-16(2)3

InchiKey: BYVYECTVTQCHMT-UHFFFAOYSA-N

Formula: C21H28O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccc(CCCC)cc1

Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
gf	272.01	kJ/mol	Joback Method
hf	-119.13	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.180		Crippen Method
mcvol	277.530	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2202.60		NIST Webbook
tb	792.51	K	Joback Method
tc	1007.83	K	Joback Method
tf	497.91	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.81	J/mol×K	792.51	Joback Method
cpg	828.92	J/mol×K	828.40	Joback Method
cpg	845.84	J/mol×K	864.28	Joback Method
cpg	861.61	J/mol×K	900.17	Joback Method
cpg	876.29	J/mol×K	936.05	Joback Method
cpg	889.91	J/mol×K	971.94	Joback Method
cpg	902.53	J/mol×K	1007.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292525&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
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