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
hfus	40.07	kJ/mol	Joback Method
logp	5.180		Crippen Method
mcvol	277.530	ml/mol	McGowan Method
rinpol	2202.60		NIST Webbook
rinpol	2202.60		NIST Webbook
tf	289.17	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point