4-Butylbenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C22H30O2/c1-6-8-10-19-12-14-20(15-13-19)22(23)24-21(16-11-17(3)4)18(5)9

InchiKey: MSZYPLUSJWKCEC-UHFFFAOYSA-N

Formula: C22H30O2

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

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	280.43	kJ/mol	Joback Method
hf	-139.77	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.570		Crippen Method
mcvol	291.620	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2288.30		NIST Webbook
rinpol	2288.30		NIST Webbook
tb	815.39	K	Joback Method
tc	1028.76	K	Joback Method
tf	509.18	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.33	J/mol×K	815.39	Joback Method
cpg	887.56	J/mol×K	850.95	Joback Method
cpg	904.59	J/mol×K	886.51	Joback Method
cpg	920.46	J/mol×K	922.08	Joback Method
cpg	935.23	J/mol×K	957.64	Joback Method
cpg	948.95	J/mol×K	993.20	Joback Method
cpg	961.66	J/mol×K	1028.76	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=U292526&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
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