4-Butylbenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C20H28O2/c1-5-7-9-17-11-13-18(14-12-17)20(21)22-19(10-8-6-2)15-16(3)4/h1

InchiKey: MHZZLZDIBWJACG-UHFFFAOYSA-N

Formula: C20H28O2

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

Mol. weight [g/mol]: 300.44

Physical Properties

Property code	Value	Unit	Source
gf	184.30	kJ/mol	Joback Method
hf	-214.13	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.014		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2160.30		NIST Webbook
tb	773.07	K	Joback Method
tc	984.92	K	Joback Method
tf	502.36	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.37	J/mol×K	773.07	Joback Method
cpg	797.60	J/mol×K	808.38	Joback Method
cpg	814.65	J/mol×K	843.69	Joback Method
cpg	830.57	J/mol×K	878.99	Joback Method
cpg	845.40	J/mol×K	914.30	Joback Method
cpg	859.17	J/mol×K	949.61	Joback Method
cpg	871.91	J/mol×K	984.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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