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
hfus	40.07	kJ/mol	Joback Method
logp	5.014		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
rinpol	2160.30		NIST Webbook
tf	262.39	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292524&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

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