4-butylbenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C17H22O2/c1-4-7-9-14-10-12-15(13-11-14)17(18)19-16(6-3)8-5-2/h10-13,16H
InchiKey: DQBGJHYNOMRKSL-UHFFFAOYSA-N
Formula: C17H22O2
SMILES: CC#CC(CC)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
hfus	35.82	kJ/mol	Joback Method
ie	8.91	eV	Cheméo Relay (1.0)
logp	3.988		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	585.85	K	Cheméo Relay (1.0)
tf	286.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.40	J/mol×K	704.87	Joback Method
cpg	627.65	J/mol×K	740.99	Joback Method
cpg	643.82	J/mol×K	777.12	Joback Method
cpg	658.95	J/mol×K	813.24	Joback Method
cpg	673.08	J/mol×K	849.37	Joback Method
cpg	686.22	J/mol×K	885.49	Joback Method
cpg	698.41	J/mol×K	921.61	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292522&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):	
Cheméo Relay (1.0, beta):	

Legend

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