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
gf	161.48	kJ/mol	Joback Method
hf	-146.93	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.988		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1976.00		NIST Webbook
tb	704.87	K	Joback Method
tc	921.61	K	Joback Method
tf	483.55	K	Joback Method
vc	0.860	m3/kmol	Joback Method

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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