4-Butylbenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C16H18O2/c1-3-5-7-13-18-16(17)15-11-9-14(10-12-15)8-6-4-2/h1,5,7,9-12H,4
InchiKey: JKKNXQJVFQVSHN-FNORWQNLSA-N
Formula: C16H18O2
SMILES: C#CC=CCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	255.99	kJ/mol	Joback Method
hf	15.81	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.375		Crippen Method
mcvol	207.080	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1953.90		NIST Webbook
rinpol	1953.90		NIST Webbook
tb	667.71	K	Joback Method
tc	882.93	K	Joback Method
tf	423.07	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.93	J/mol×K	667.71	Joback Method
cpg	546.48	J/mol×K	703.58	Joback Method
cpg	561.06	J/mol×K	739.45	Joback Method
cpg	574.71	J/mol×K	775.32	Joback Method
cpg	587.50	J/mol×K	811.19	Joback Method
cpg	599.47	J/mol×K	847.06	Joback Method
cpg	610.67	J/mol×K	882.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292521&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

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