4-Ethylbenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C13H14O2/c1-4-10(3)15-13(14)12-8-6-11(5-2)7-9-12/h1,6-10H,5H2,2-3H3
InchiKey: NUHIVOBFSLBHKA-UHFFFAOYSA-N
Formula: C13H14O2
SMILES: C#CC(C)OC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	148.07	kJ/mol	Joback Method
hf	-44.77	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.428		Crippen Method
mcvol	169.110	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1521.10		NIST Webbook
rinpol	1521.10		NIST Webbook
tb	594.47	K	Joback Method
tc	816.64	K	Joback Method
tf	379.34	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.99	J/mol×K	594.47	Joback Method
cpg	416.73	J/mol×K	631.50	Joback Method
cpg	430.56	J/mol×K	668.53	Joback Method
cpg	443.52	J/mol×K	705.56	Joback Method
cpg	455.63	J/mol×K	742.59	Joback Method
cpg	466.92	J/mol×K	779.62	Joback Method
cpg	477.42	J/mol×K	816.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292540&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