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

Inchi: InChI=1S/C15H18O2/c1-4-7-14(6-3)17-15(16)13-10-8-12(5-2)9-11-13/h8-11,14H,5-6H2,1
InchiKey: ILJACNQHGIRAAX-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: CC#CC(CC)OC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	144.64	kJ/mol	Joback Method
hf	-105.65	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.208		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1782.10		NIST Webbook
tb	659.11	K	Joback Method
tc	883.34	K	Joback Method
tf	461.01	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.01	J/mol×K	659.11	Joback Method
cpg	520.47	J/mol×K	696.48	Joback Method
cpg	535.90	J/mol×K	733.85	Joback Method
cpg	550.33	J/mol×K	771.23	Joback Method
cpg	563.80	J/mol×K	808.60	Joback Method
cpg	576.33	J/mol×K	845.97	Joback Method
cpg	587.94	J/mol×K	883.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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