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

Inchi: InChI=1S/C14H14O2/c1-3-5-6-11-16-14(15)13-9-7-12(4-2)8-10-13/h1,5-10H,4,11H2,2H3
InchiKey: RUVVJERLIGXFDS-AATRIKPKSA-N
Formula: C14H14O2
SMILES: C#CC=CCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	239.15	kJ/mol	Joback Method
hf	57.09	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.595		Crippen Method
mcvol	178.900	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1758.80		NIST Webbook
rinpol	1758.80		NIST Webbook
tb	621.95	K	Joback Method
tc	844.80	K	Joback Method
tf	400.53	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.62	J/mol×K	621.95	Joback Method
cpg	444.08	J/mol×K	659.09	Joback Method
cpg	457.62	J/mol×K	696.23	Joback Method
cpg	470.26	J/mol×K	733.38	Joback Method
cpg	482.06	J/mol×K	770.52	Joback Method
cpg	493.07	J/mol×K	807.66	Joback Method
cpg	503.34	J/mol×K	844.80	Joback Method

Sources

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=U292542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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