p-Anisic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H12O3/c1-3-4-5-10-16-13(14)11-6-8-12(15-2)9-7-11/h1,4-9H,10H2,2H3
InchiKey: FWBPOUCFYDTKMC-UHFFFAOYSA-N
Formula: C13H12O3
SMILES: C#CC=CCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
gf	125.73	kJ/mol	Joback Method
hf	-54.49	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.041		Crippen Method
mcvol	170.680	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
tb	621.49	K	Joback Method
tc	845.55	K	Joback Method
tf	411.49	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.39	J/mol×K	621.49	Joback Method
cpg	418.89	J/mol×K	658.83	Joback Method
cpg	431.53	J/mol×K	696.18	Joback Method
cpg	443.34	J/mol×K	733.52	Joback Method
cpg	454.36	J/mol×K	770.87	Joback Method
cpg	464.61	J/mol×K	808.21	Joback Method
cpg	474.12	J/mol×K	845.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299193&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