p-Anisic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H22O3/c1-13(2)6-9-17(12-14(3)4)21-18(19)15-7-10-16(20-5)11-8-15/h7-8,

InchiKey: BNVUAFGNMYVRML-UHFFFAOYSA-N

Formula: C18H22O3

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccc(OC)cc1

Mol. weight [g/mol]: 286.37

Physical Properties

Property code	Value	Unit	Source
gf	141.75	kJ/mol	Joback Method
hf	-189.43	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	70.95	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.846		Crippen Method
mcvol	241.130	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	746.29	K	Joback Method
tc	968.15	K	Joback Method
tf	486.33	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.11	J/mol×K	746.29	Joback Method
cpg	686.17	J/mol×K	783.27	Joback Method
cpg	702.07	J/mol×K	820.24	Joback Method
cpg	716.83	J/mol×K	857.22	Joback Method
cpg	730.47	J/mol×K	894.20	Joback Method
cpg	743.03	J/mol×K	931.18	Joback Method
cpg	754.52	J/mol×K	968.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299197&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