p-Anisic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H24O3/c1-6-7-15(4)18(13-8-14(2)3)22-19(20)16-9-11-17(21-5)12-10-16/h9
InchiKey: ZXNBGPUXUJMIHT-UHFFFAOYSA-N
Formula: C19H24O3
SMILES: C=C(C)C#CC(OC(=O)c1ccc(OC)cc1)C(C)CCC
Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	150.17	kJ/mol	Joback Method
hf	-210.07	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	73.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.236		Crippen Method
mcvol	255.220	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2119.00		NIST Webbook
rinpol	2119.00		NIST Webbook
tb	769.17	K	Joback Method
tc	987.91	K	Joback Method
tf	497.60	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.20	J/mol×K	769.17	Joback Method
cpg	742.46	J/mol×K	805.63	Joback Method
cpg	758.54	J/mol×K	842.08	Joback Method
cpg	773.46	J/mol×K	878.54	Joback Method
cpg	787.25	J/mol×K	914.99	Joback Method
cpg	799.94	J/mol×K	951.45	Joback Method
cpg	811.56	J/mol×K	987.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299198&Units=SI

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