m-Anisic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H22O3/c1-5-6-9-16(11-13(2)3)20-17(18)14-8-7-10-15(12-14)19-4/h7-8,10,
InchiKey: BTRQGPIQAUUDNO-UHFFFAOYSA-N
Formula: C17H22O3
SMILES: CCC#CC(CC(C)C)OC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	54.04	kJ/mol	Joback Method
hf	-284.43	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.680		Crippen Method
mcvol	231.340	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1975.80		NIST Webbook
rinpol	1975.80		NIST Webbook
tb	726.85	K	Joback Method
tc	945.11	K	Joback Method
tf	490.78	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.93	J/mol×K	726.85	Joback Method
cpg	656.04	J/mol×K	763.23	Joback Method
cpg	672.03	J/mol×K	799.60	Joback Method
cpg	686.92	J/mol×K	835.98	Joback Method
cpg	700.73	J/mol×K	872.36	Joback Method
cpg	713.46	J/mol×K	908.73	Joback Method
cpg	725.13	J/mol×K	945.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292596&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

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