m-anisic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H24O3/c1-6-8-15(4)18(12-11-14(2)3)22-19(20)16-9-7-10-17(13-16)21-5/h7
InchiKey: UFUDEWWCCJOFQT-UHFFFAOYSA-N
Formula: C19H24O3
SMILES: C=C(C)C#CC(OC(=O)c1cccc(OC)c1)C(C)CCC
Mol. weight [g/mol]: 300.40

Physical Properties

Property code	Value	Unit	Source
hfus	36.08	kJ/mol	Joback Method
ie	8.33	eV	Cheméo Relay (1.0)
logp	4.236		Crippen Method
mcvol	255.220	ml/mol	McGowan Method
rinpol	2092.50		NIST Webbook
tb	609.14	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292597&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature