m-Anisic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C20H28O3/c1-3-4-5-6-7-8-9-10-11-12-16-23-20(21)18-14-13-15-19(17-18)22-2
InchiKey: OYYUOQHWUGTEQY-UHFFFAOYSA-N
Formula: C20H28O3
SMILES: CCC#CCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	84.18	kJ/mol	Joback Method
hf	-335.79	kJ/mol	Joback Method
hfus	48.30	kJ/mol	Joback Method
hvap	76.77	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.996		Crippen Method
mcvol	273.610	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2465.50		NIST Webbook
rinpol	2465.50		NIST Webbook
tb	796.37	K	Joback Method
tc	1001.55	K	Joback Method
tf	554.59	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.92	J/mol×K	796.37	Joback Method
cpg	825.15	J/mol×K	830.57	Joback Method
cpg	841.26	J/mol×K	864.76	Joback Method
cpg	856.29	J/mol×K	898.96	Joback Method
cpg	870.23	J/mol×K	933.16	Joback Method
cpg	883.13	J/mol×K	967.35	Joback Method
cpg	894.99	J/mol×K	1001.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292256&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