m-Anisic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H16O3/c1-4-7-12(5-2)17-14(15)11-8-6-9-13(10-11)16-3/h6,8-10,12H,5H2,1
InchiKey: BRKFXYDZNLLXEI-UHFFFAOYSA-N
Formula: C14H16O3
SMILES: CC#CC(CC)OC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
gf	31.22	kJ/mol	Joback Method
hf	-217.23	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	63.03	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.654		Crippen Method
mcvol	189.070	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1793.40		NIST Webbook
rinpol	1793.40		NIST Webbook
tb	658.65	K	Joback Method
tc	884.05	K	Joback Method
tf	471.97	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.71	J/mol×K	658.65	Joback Method
cpg	494.28	J/mol×K	696.22	Joback Method
cpg	508.90	J/mol×K	733.78	Joback Method
cpg	522.56	J/mol×K	771.35	Joback Method
cpg	535.28	J/mol×K	808.92	Joback Method
cpg	547.05	J/mol×K	846.48	Joback Method
cpg	557.89	J/mol×K	884.05	Joback Method

Sources

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=U292594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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