m-Anisic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H30O3/c1-3-4-5-6-7-8-9-10-11-12-13-17-24-21(22)19-15-14-16-20(18-19)2
InchiKey: MFXYRCBEMYFFSU-UHFFFAOYSA-N
Formula: C21H30O3
SMILES: CCCCCCCCCCC#CCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	92.60	kJ/mol	Joback Method
hf	-356.43	kJ/mol	Joback Method
hfus	50.89	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.386		Crippen Method
mcvol	287.700	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2535.50		NIST Webbook
rinpol	2535.50		NIST Webbook
tb	819.25	K	Joback Method
tc	1023.62	K	Joback Method
tf	565.86	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.52	J/mol×K	819.25	Joback Method
cpg	883.93	J/mol×K	853.31	Joback Method
cpg	900.19	J/mol×K	887.37	Joback Method
cpg	915.32	J/mol×K	921.44	Joback Method
cpg	929.36	J/mol×K	955.50	Joback Method
cpg	942.31	J/mol×K	989.56	Joback Method
cpg	954.21	J/mol×K	1023.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292599&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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