

o-anisic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H30O3/c1-3-4-5-6-7-8-9-10-11-12-15-18-24-21(22)19-16-13-14-17-20(19)2
InchiKey: AHLTWCUDPVNCME-UHFFFAOYSA-N
Formula: C21H30O3
SMILES: CCCCCCCCCC#CCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 330.47

Physical Properties

Property code	Value	Unit	Source
hf	-405.69	kJ/mol	Cheméo Relay (1.0)
hfus	50.89	kJ/mol	Joback Method
hvap	106.32	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.53		Cheméo Relay (1.0)
logp	5.386		Crippen Method
mcvol	287.700	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2515.80		NIST Webbook
rinpol	2515.80		NIST Webbook
tb	631.95	K	Cheméo Relay (1.0)
tf	292.68	K	Cheméo Relay (1.0)

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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292579&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point

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