

m-Anisic acid, undec-2-enyl ester

Inchi:	InChI=1S/C19H28O3/c1-3-4-5-6-7-8-9-10-11-15-22-19(20)17-13-12-14-18(16-17)21-2/h
InchiKey:	VAGYOTSVLFBXDK-ZHACJKMWSA-N
Formula:	C19H28O3
SMILES:	CCCCCCCC=CCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	304.42

Physical Properties

Property code	Value	Unit	Source
gf	-46.82	kJ/mol	Joback Method
hf	-470.23	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	72.35	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.159		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinsol	2338.40		NIST Webbook
tb	768.65	K	Joback Method
tc	965.66	K	Joback Method
tf	432.14	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.64	J/molxK	768.65	Joback Method
cpg	849.17	J/molxK	932.83	Joback Method
cpg	835.97	J/molxK	899.99	Joback Method
cpg	821.84	J/molxK	867.16	Joback Method
cpg	806.77	J/molxK	834.32	Joback Method
cpg	790.71	J/molxK	801.49	Joback Method
cpg	861.48	J/molxK	965.66	Joback Method
dvisc	0.0000561	Paxs	768.65	Joback Method
dvisc	0.0000728	Paxs	712.57	Joback Method

dvisc	0.0000989	Paxs	656.48	Joback Method
dvisc	0.0001421	Paxs	600.39	Joback Method
dvisc	0.0002200	Paxs	544.31	Joback Method
dvisc	0.0003767	Paxs	488.23	Joback Method
dvisc	0.0007416	Paxs	432.14	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=U292598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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