

Benzoic acid, 3-methoxy-, undecyl ester

Other names:	m-Anisic acid, undecyl ester
Inchi:	InChI=1S/C19H30O3/c1-3-4-5-6-7-8-9-10-11-15-22-19(20)17-13-12-14-18(16-17)21-2/h1
InchiKey:	NECXTBYDKQTNTP-UHFFFAOYSA-N
Formula:	C19H30O3
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	306.44
CAS:	69833-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-127.04	kJ/mol	Joback Method
hf	-587.45	kJ/mol	Joback Method
hfus	42.59	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.383		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2332.80		NIST Webbook
rinpol	2332.80		NIST Webbook
tb	764.49	K	Joback Method
tc	956.45	K	Joback Method
tf	437.22	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.09	J/molxK	764.49	Joback Method
cpg	815.64	J/molxK	796.48	Joback Method
cpg	832.16	J/molxK	828.48	Joback Method
cpg	847.67	J/molxK	860.47	Joback Method
cpg	862.20	J/molxK	892.46	Joback Method
cpg	875.75	J/molxK	924.45	Joback Method

cpg	888.35	J/mol×K	956.45	Joback Method
dvisc	0.0008021	Paxs	437.22	Joback Method
dvisc	0.0004177	Paxs	491.76	Joback Method
dvisc	0.0002478	Paxs	546.31	Joback Method
dvisc	0.0001616	Paxs	600.86	Joback Method
dvisc	0.0001132	Paxs	655.40	Joback Method
dvisc	0.0000837	Paxs	709.94	Joback Method
dvisc	0.0000646	Paxs	764.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C69833358&Units=SI

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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