Benzoic acid, 3-methoxy-, pentadecyl ester

Other names:	m-Methoxybenzoic acid, pentadecyl ester
Inchi:	InChI=1S/C23H38O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-26-23(24)21-17-16-18-22(2
InchiKey:	JVOYLBAHXOMJHN-UHFFFAOYSA-N
Formula:	C23H38O3
SMILES:	CCCCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	362.55
CAS:	56954-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-93.36	kJ/mol	Joback Method
hf	-670.01	kJ/mol	Joback Method
hfus	52.95	kJ/mol	Joback Method
hvap	81.30	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.943		Crippen Method
mcvol	324.480	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	2686.70		NIST Webbook
rinpol	2686.70		NIST Webbook
tb	856.01	K	Joback Method
tc	1052.14	K	Joback Method
tf	482.30	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.63	J/mol×K	856.01	Joback Method
cpg	1056.16	J/mol×K	888.70	Joback Method
cpg	1073.48	J/mol×K	921.39	Joback Method
cpg	1089.63	J/mol×K	954.07	Joback Method
cpg	1104.62	J/mol×K	986.76	Joback Method
cpg	1118.50	J/mol×K	1019.45	Joback Method

cpg	1131.29	J/mol×K	1052.14	Joback Method
dvisc	0.0005394	Pa×s	482.30	Joback Method
dvisc	0.0002681	Pa×s	544.59	Joback Method
dvisc	0.0001538	Pa×s	606.87	Joback Method
dvisc	0.0000978	Pa×s	669.15	Joback Method
dvisc	0.0000672	Pa×s	731.44	Joback Method
dvisc	0.0000490	Pa×s	793.72	Joback Method
dvisc	0.0000374	Pa×s	856.01	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=C56954757&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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