Benzoic acid, 3-methoxy-, tridecyl ester

Other names: m-Methoxybenzoic acid, tridecyl ester
Inchi: InChI=1S/C21H34O3/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: BCRGROQQCHLFHT-UHFFFAOYSA-N
Formula: C21H34O3
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 334.49
CAS: 69833-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-110.20	kJ/mol	Joback Method
hf	-628.73	kJ/mol	Joback Method
hfus	47.77	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.163		Crippen Method
mcvol	296.300	ml/mol	McGowan Method
pc	1198.13	kPa	Joback Method
rinpol	2515.50		NIST Webbook
tb	810.25	K	Joback Method
tc	1002.94	K	Joback Method
tf	459.76	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.24	J/mol×K	810.25	Joback Method
cpg	995.58	J/mol×K	970.82	Joback Method
cpg	981.83	J/mol×K	938.71	Joback Method
cpg	967.05	J/mol×K	906.59	Joback Method
cpg	951.20	J/mol×K	874.48	Joback Method
cpg	934.27	J/mol×K	842.36	Joback Method
cpg	1008.32	J/mol×K	1002.94	Joback Method

dvisc	0.0000494	Pa×s	810.25	Joback Method
dvisc	0.0000644	Pa×s	751.84	Joback Method
dvisc	0.0000878	Pa×s	693.42	Joback Method
dvisc	0.0001266	Pa×s	635.00	Joback Method
dvisc	0.0001967	Pa×s	576.59	Joback Method
dvisc	0.0003374	Pa×s	518.17	Joback Method
dvisc	0.0006638	Pa×s	459.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69833370&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