

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)
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/molxK	810.25	Joback Method
cpg	934.27	J/molxK	842.36	Joback Method
cpg	951.20	J/molxK	874.48	Joback Method
cpg	967.05	J/molxK	906.59	Joback Method
cpg	981.83	J/molxK	938.71	Joback Method
cpg	995.58	J/molxK	970.82	Joback Method
cpg	1008.32	J/molxK	1002.94	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69833370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mvol:	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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