

m-Methoxybenzoic acid, hexadecyl ester

Inchi: InChI=1S/C24H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-27-24(25)22-18-17-19-2
InchiKey: GTIJNPYMBMWTEW-UHFFFAOYSA-N
Formula: C24H40O3
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 376.57
CAS: 111722-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-84.94	kJ/mol	Joback Method
hf	-690.65	kJ/mol	Joback Method
hfus	55.54	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.333		Crippen Method
mcvol	338.570	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	2768.80		NIST Webbook
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tb	878.89	K	Joback Method
tc	1077.89	K	Joback Method
tf	493.57	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.37	J/molxK	878.89	Joback Method
cpg	1118.17	J/molxK	912.06	Joback Method
cpg	1135.70	J/molxK	945.22	Joback Method
cpg	1152.00	J/molxK	978.39	Joback Method
cpg	1167.09	J/molxK	1011.56	Joback Method
cpg	1181.02	J/molxK	1044.73	Joback Method
cpg	1193.81	J/molxK	1077.89	Joback Method

dvisc	0.0004833	Paxs	493.57	Joback Method
dvisc	0.0002376	Paxs	557.79	Joback Method
dvisc	0.0001353	Paxs	622.01	Joback Method
dvisc	0.0000856	Paxs	686.23	Joback Method
dvisc	0.0000586	Paxs	750.45	Joback Method
dvisc	0.0000425	Paxs	814.67	Joback Method
dvisc	0.0000324	Paxs	878.89	Joback Method

Sources

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=C111722113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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