Benzoic acid, 3-methoxy-, decyl ester

Other names: m-Methoxybenzoic acid, decyl ester
Inchi: InChI=1S/C18H28O3/c1-3-4-5-6-7-8-9-10-14-21-18(19)16-12-11-13-17(15-16)20-2/h11-1
InchiKey: KNUKZBZOCHMAEK-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 292.41
CAS: 69833-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-135.46	kJ/mol	Joback Method
hf	-566.81	kJ/mol	Joback Method
hfus	40.00	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.993		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2237.80		NIST Webbook
rinpol	2237.80		NIST Webbook
tb	741.61	K	Joback Method
tc	934.08	K	Joback Method
tf	425.95	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.43	J/mol×K	741.61	Joback Method
cpg	817.09	J/mol×K	902.00	Joback Method
cpg	803.67	J/mol×K	869.93	Joback Method
cpg	789.31	J/mol×K	837.85	Joback Method
cpg	774.00	J/mol×K	805.77	Joback Method
cpg	757.71	J/mol×K	773.69	Joback Method

cpg	829.58	J/mol×K	934.08	Joback Method
dvisc	0.0000735	Pa×s	741.61	Joback Method
dvisc	0.0000949	Pa×s	689.00	Joback Method
dvisc	0.0001278	Pa×s	636.39	Joback Method
dvisc	0.0001815	Pa×s	583.78	Joback Method
dvisc	0.0002763	Pa×s	531.17	Joback Method
dvisc	0.0004615	Pa×s	478.56	Joback Method
dvisc	0.0008747	Pa×s	425.95	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=C69833381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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