Benzoic acid, dec-2-yl ester

Inchi: InChI=1S/C17H26O2/c1-3-4-5-6-7-9-12-15(2)19-17(18)16-13-10-8-11-14-16/h8,10-11,13
InchiKey: WPQGCBLKSNYZOU-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCCCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-31.69	kJ/mol	Joback Method
hf	-407.76	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.982		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	1914.00		NIST Webbook
tb	690.89	K	Joback Method
tc	887.37	K	Joback Method
tf	364.93	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.33	J/mol×K	690.89	Joback Method
cpg	673.13	J/mol×K	723.64	Joback Method
cpg	689.91	J/mol×K	756.38	Joback Method
cpg	705.70	J/mol×K	789.13	Joback Method
cpg	720.53	J/mol×K	821.87	Joback Method
cpg	734.45	J/mol×K	854.62	Joback Method
cpg	747.47	J/mol×K	887.37	Joback Method
dvisc	0.0020940	Pa×s	364.93	Joback Method
dvisc	0.0009088	Pa×s	419.26	Joback Method

dvisc	0.0004777	Pa×s	473.58	Joback Method
dvisc	0.0002866	Pa×s	527.91	Joback Method
dvisc	0.0001892	Pa×s	582.24	Joback Method
dvisc	0.0001340	Pa×s	636.56	Joback Method
dvisc	0.0001003	Pa×s	690.89	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=U367897&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