4-O-Acetylthebaol

Inchi: InChI=1S/C18H16O4/c1-11(19)22-18-16(21-3)9-7-13-5-4-12-6-8-14(20-2)10-15(12)17(13
InchiKey: RIUJHBDYSWDQNC-UHFFFAOYSA-N
Formula: C18H16O4
SMILES: COc1ccc2ccc3ccc(OC)c(OC(C)=O)c3c2c1
Mol. weight [g/mol]: 296.32

Physical Properties

Property code	Value	Unit	Source
gf	-56.05	kJ/mol	Joback Method
hf	-351.30	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	3.935		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2591.00		NIST Webbook
tb	816.93	K	Joback Method
tc	1048.62	K	Joback Method
tf	551.14	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.11	J/mol×K	816.93	Joback Method
cpg	682.65	J/mol×K	1010.00	Joback Method
cpg	672.99	J/mol×K	971.39	Joback Method
cpg	662.45	J/mol×K	932.77	Joback Method
cpg	650.99	J/mol×K	894.16	Joback Method
cpg	638.55	J/mol×K	855.54	Joback Method
cpg	691.46	J/mol×K	1048.62	Joback Method
dvisc	0.0002161	Pa×s	816.93	Joback Method
dvisc	0.0002461	Pa×s	772.63	Joback Method

dvisc	0.0002847	Pa×s	728.33	Joback Method
dvisc	0.0003356	Pa×s	684.04	Joback Method
dvisc	0.0004048	Pa×s	639.74	Joback Method
dvisc	0.0005020	Pa×s	595.44	Joback Method
dvisc	0.0006445	Pa×s	551.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330793&Units=SI
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

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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