

trans-Acenaphthen-1,2-diol, diacetate

Inchi:	InChI=1S/C16H14O4/c1-9(17)19-15-12-7-3-5-11-6-4-8-13(14(11)12)16(15)20-10(2)18/h3
InchiKey:	AFKBNGVZYDAUNA-HZPDHXFCSA-N
Formula:	C16H14O4
SMILES:	CC(=O)OC1c2cccc3cccc(c23)C1OC(C)=O
Mol. weight [g/mol]:	270.28

Physical Properties

Property code	Value	Unit	Source
gf	-119.06	kJ/mol	Joback Method
hf	-399.89	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.062		Crippen Method
mvol	197.100	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	771.48	K	Joback Method
tc	1000.55	K	Joback Method
tf	515.78	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.65	J/molxK	771.48	Joback Method
cpg	575.03	J/molxK	809.66	Joback Method
cpg	587.47	J/molxK	847.84	Joback Method
cpg	599.04	J/molxK	886.02	Joback Method
cpg	609.80	J/molxK	924.20	Joback Method
cpg	619.82	J/molxK	962.37	Joback Method
cpg	629.18	J/molxK	1000.55	Joback Method
dvisc	0.0019723	Paxs	515.78	Joback Method

dvisc	0.0016490	Paxs	558.40	Joback Method
dvisc	0.0014141	Paxs	601.01	Joback Method
dvisc	0.0012376	Paxs	643.63	Joback Method
dvisc	0.0011012	Paxs	686.25	Joback Method
dvisc	0.0009934	Paxs	728.86	Joback Method
dvisc	0.0009063	Paxs	771.48	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=R109678&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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