Anthracen-2-ol, acetate

Inchi: InChI=1S/C16H12O2/c1-11(17)18-16-7-6-14-8-12-4-2-3-5-13(12)9-15(14)10-16/h2-10H,1
InchiKey: AKUJZWDYELFGNV-UHFFFAOYSA-N
Formula: C16H12O2
SMILES: CC(=O)Oc1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	156.37	kJ/mol	Joback Method
hf	-22.64	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.918		Crippen Method
mcvol	181.060	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
tb	716.37	K	Joback Method
tc	961.80	K	Joback Method
tf	459.10	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.90	J/mol×K	716.37	Joback Method
cpg	528.42	J/mol×K	920.90	Joback Method
cpg	518.39	J/mol×K	879.99	Joback Method
cpg	507.63	J/mol×K	839.09	Joback Method
cpg	496.03	J/mol×K	798.18	Joback Method
cpg	483.48	J/mol×K	757.28	Joback Method
cpg	537.82	J/mol×K	961.80	Joback Method
dvisc	0.0003989	Pa×s	716.37	Joback Method

dvisc	0.0004567	Pa×s	673.49	Joback Method
dvisc	0.0005325	Pa×s	630.61	Joback Method
dvisc	0.0006349	Pa×s	587.74	Joback Method
dvisc	0.0007783	Pa×s	544.86	Joback Method
dvisc	0.0009879	Pa×s	501.98	Joback Method
dvisc	0.0013111	Pa×s	459.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109207&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

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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