

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
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tb	716.37	K	Joback Method
tc	961.80	K	Joback Method
tf	459.10	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.90	J/molxK	716.37	Joback Method
cpg	483.48	J/molxK	757.28	Joback Method
cpg	496.03	J/molxK	798.18	Joback Method
cpg	507.63	J/molxK	839.09	Joback Method
cpg	518.39	J/molxK	879.99	Joback Method
cpg	528.42	J/molxK	920.90	Joback Method
cpg	537.82	J/molxK	961.80	Joback Method
dvisc	0.0013111	Paxs	459.10	Joback Method

dvisc	0.0009879	Paxs	501.98	Joback Method
dvisc	0.0007783	Paxs	544.86	Joback Method
dvisc	0.0006349	Paxs	587.74	Joback Method
dvisc	0.0005325	Paxs	630.61	Joback Method
dvisc	0.0004567	Paxs	673.49	Joback Method
dvisc	0.0003989	Paxs	716.37	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=R109207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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