

Anthralin, O,O',O''-tri(acetyl)-

Inchi:	InChI=1S/C20H16O6/c1-11(21)24-16-8-4-6-14-10-15-7-5-9-17(25-12(2)22)19(15)20(18)(
InchiKey:	IPWOSICBVUXMML-UHFFFAOYSA-N
Formula:	C20H16O6
SMILES:	CC(=O)Oc1cccc2cc3cccc(OC(C)=O)c3c(OC(C)=O)c12
Mol. weight [g/mol]:	352.34

Physical Properties

Property code	Value	Unit	Source
gf	-297.05	kJ/mol	Joback Method
hf	-617.74	kJ/mol	Joback Method
hfus	42.44	kJ/mol	Joback Method
hvap	95.79	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	3.769		Crippen Method
mcvol	252.300	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinsol	2802.00		NIST Webbook
tb	970.43	K	Joback Method
tc	1208.79	K	Joback Method
tf	673.54	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.67	J/molxK	970.43	Joback Method
cpg	795.05	J/molxK	1169.06	Joback Method
cpg	788.72	J/molxK	1129.34	Joback Method
cpg	781.46	J/molxK	1089.61	Joback Method
cpg	773.23	J/molxK	1049.88	Joback Method
cpg	763.98	J/molxK	1010.16	Joback Method
cpg	800.50	J/molxK	1208.79	Joback Method
dvisc	0.0001798	Paxs	970.43	Joback Method
dvisc	0.0002069	Paxs	920.95	Joback Method

dvisc	0.0002418	Paxs	871.47	Joback Method
dvisc	0.0002881	Paxs	821.99	Joback Method
dvisc	0.0003509	Paxs	772.50	Joback Method
dvisc	0.0004391	Paxs	723.02	Joback Method
dvisc	0.0005679	Paxs	673.54	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=U374775&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

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