9-anthrol

Other names: 1-anthranol
Inchi: InChI=1S/C14H10O/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9,15H
InchiKey: AUKRYONWZHRJRE-UHFFFAOYSA-N
Formula: C14H10O
SMILES: Oc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	228.46	kJ/mol	Joback Method
hf	97.60	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-4.73		Estimated Solubility Method
log10ws	-4.73		Aqueous Solubility Prediction Method
logp	3.699		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	669.96	K	Joback Method
tc	932.17	K	Joback Method
tf	463.60	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.08	J/mol×K	669.96	Joback Method
cpg	393.60	J/mol×K	713.66	Joback Method
cpg	405.10	J/mol×K	757.36	Joback Method
cpg	415.82	J/mol×K	801.06	Joback Method
cpg	425.98	J/mol×K	844.77	Joback Method
cpg	435.80	J/mol×K	888.47	Joback Method

cpg	445.51	J/mol×K	932.17	Joback Method
dvisc	0.0006150	Pa×s	463.60	Joback Method
dvisc	0.0003636	Pa×s	497.99	Joback Method
dvisc	0.0002300	Pa×s	532.39	Joback Method
dvisc	0.0001539	Pa×s	566.78	Joback Method
dvisc	0.0001078	Pa×s	601.17	Joback Method
dvisc	0.0000784	Pa×s	635.57	Joback Method
dvisc	0.0000590	Pa×s	669.96	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume