2,3-Naphthalenediol diacetate

Other names: 3-(Acetyloxy)-2-naphthyl acetate
2,3-Dihydroxynaphthalene, diacetate
Inchi: InChI=1S/C14H12O4/c1-9(15)17-13-7-11-5-3-4-6-12(11)8-14(13)18-10(2)16/h3-8H,1-2H
InchiKey: CNUNETLANGTFDD-UHFFFAOYSA-N
Formula: C14H12O4
SMILES: CC(=O)Oc1cc2ccccc2cc1OC(C)=O
Mol. weight [g/mol]: 244.24
CAS: 22426-46-6

Physical Properties

Property code	Value	Unit	Source
gf	-201.04	kJ/mol	Joback Method
hf	-417.23	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	70.31	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.690		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1938.40		NIST Webbook
tb	727.92	K	Joback Method
tc	957.77	K	Joback Method
tf	476.02	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.72	J/mol×K	727.92	Joback Method
cpg	525.12	J/mol×K	919.46	Joback Method
cpg	516.19	J/mol×K	881.15	Joback Method
cpg	506.41	J/mol×K	842.84	Joback Method
cpg	495.76	J/mol×K	804.54	Joback Method
cpg	484.21	J/mol×K	766.23	Joback Method

cpg	533.23	J/mol×K	957.77	Joback Method
dvisc	0.0002177	Pa×s	727.92	Joback Method
dvisc	0.0002576	Pa×s	685.94	Joback Method
dvisc	0.0003115	Pa×s	643.95	Joback Method
dvisc	0.0003867	Pa×s	601.97	Joback Method
dvisc	0.0004960	Pa×s	559.99	Joback Method
dvisc	0.0006624	Pa×s	518.00	Joback Method
dvisc	0.0009310	Pa×s	476.02	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22426466&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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