Benz[j]aceanthrylen-1-ol, 1,2-dihydro-3-methyl-

Other names: 1-Cholanthrenol, 3-methyl-
1-Hydroxy-3-methylcholanthrene
3-Methylcholanthren-1-ol
15-Hydroxy-20-methylcholanthrene

Inchi: InChI=1S/C21H16O/c1-12-6-7-14-10-18-15-5-3-2-4-13(15)8-9-16(18)21-19(22)11-17(12)

InchiKey: CHNZFZQGTXDBFI-UHFFFAOYSA-N

Formula: C21H16O

SMILES: Cc1ccc2cc3c(ccc4ccccc43)c3c2c1CC3O

Mol. weight [g/mol]: 284.35

CAS: 3342-98-1

Physical Properties

Property code	Value	Unit	Source
gf	446.18	kJ/mol	Joback Method
hf	202.35	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	89.27	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	5.044		Crippen Method
mcvol	219.620	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
tb	883.05	K	Joback Method
tc	1120.56	K	Joback Method
tf	595.83	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.67	J/mol×K	883.05	Joback Method
cpg	720.44	J/mol×K	1080.98	Joback Method
cpg	706.99	J/mol×K	1041.39	Joback Method
cpg	693.88	J/mol×K	1001.81	Joback Method
cpg	680.92	J/mol×K	962.22	Joback Method

cpg	667.91	J/mol×K	922.64	Joback Method
cpg	734.43	J/mol×K	1120.56	Joback Method
dvisc	0.0005337	Pa×s	883.05	Joback Method
dvisc	0.0006141	Pa×s	835.18	Joback Method
dvisc	0.0007188	Pa×s	787.31	Joback Method
dvisc	0.0008587	Pa×s	739.44	Joback Method
dvisc	0.0010514	Pa×s	691.57	Joback Method
dvisc	0.0013267	Pa×s	643.70	Joback Method
dvisc	0.0017377	Pa×s	595.83	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=C3342981&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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