Benzo(a)pyrene 4,5-oxide

Other names:	Benzo(a)pyrene 4,5-epoxide
	Benzo(1,2)pyreno(4,5-b)oxirene, 3b,4a-dihydro-
	Benz(a)pyrene 4,5-oxide
	Bp 4,5-epoxide
	Bp 4,5-oxide
	4,5-Dihydro-4,5-epoxybenzpyrene
Inchi:	InChI=1S/C20H12O/c1-2-6-13-12(4-1)10-16-18-14(13)9-8-11-5-3-7-15(17(11)18)19-20(1
InchiKey:	XGZQLNASOQVQTD-UHFFFAOYSA-N
Formula:	C20H12O
SMILES:	c1ccc2c(c1)cc1c3c2ccc2cccc(c23)C2OC12
Mol. weight [g/mol]:	268.31
CAS:	37574-47-3

Physical Properties

Property code	Value	Unit	Source
gf	583.04	kJ/mol	Joback Method
hf	339.81	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	5.272		Crippen Method
mcvol	194.670	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	788.16	K	Joback Method
tc	1046.20	K	Joback Method
tf	562.77	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.75	J/mol×K	788.16	Joback Method
cpg	570.19	J/mol×K	831.17	Joback Method
cpg	583.20	J/mol×K	874.17	Joback Method

cpg	596.09	J/mol×K	917.18	Joback Method
cpg	609.18	J/mol×K	960.19	Joback Method
cpg	622.81	J/mol×K	1003.20	Joback Method
cpg	637.28	J/mol×K	1046.20	Joback Method
dvisc	0.0129637	Pa×s	562.77	Joback Method
dvisc	0.0134267	Pa×s	600.34	Joback Method
dvisc	0.0138488	Pa×s	637.90	Joback Method
dvisc	0.0142351	Pa×s	675.47	Joback Method
dvisc	0.0145899	Pa×s	713.03	Joback Method
dvisc	0.0149166	Pa×s	750.60	Joback Method
dvisc	0.0152186	Pa×s	788.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37574473&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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