Benzo[kl]xanthene

Inchi: InChI=1S/C16H10O/c1-2-9-14-12(7-1)13-8-3-5-11-6-4-10-15(17-14)16(11)13/h1-10H
InchiKey: QKOSFCWXOIAFTO-UHFFFAOYSA-N
Formula: C16H10O
SMILES: c1ccc2c(c1)Oc1cccc3cccc-2c13
Mol. weight [g/mol]: 218.25
CAS: 200-23-7

Physical Properties

Property code	Value	Unit	Source
gf	392.96	kJ/mol	Joback Method
hf	229.61	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.612		Crippen Method
mcvol	164.330	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	361.60		NIST Webbook
rinpol	361.38		NIST Webbook
rinpol	360.96		NIST Webbook
rinpol	360.96		NIST Webbook
rinpol	359.77		NIST Webbook
rinpol	361.38		NIST Webbook
rinpol	359.85		NIST Webbook
tb	682.58	K	Joback Method
tc	943.00	K	Joback Method
tf	448.97	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.92	J/mol×K	682.58	Joback Method
cpg	474.35	J/mol×K	899.59	Joback Method

cpg	464.27	J/mol×K	856.19	Joback Method
cpg	453.69	J/mol×K	812.79	Joback Method
cpg	442.41	J/mol×K	769.39	Joback Method
cpg	430.22	J/mol×K	725.98	Joback Method
cpg	484.13	J/mol×K	943.00	Joback Method
dvisc	0.0010034	Pa×s	682.58	Joback Method
dvisc	0.0010930	Pa×s	643.64	Joback Method
dvisc	0.0012037	Pa×s	604.71	Joback Method
dvisc	0.0013433	Pa×s	565.77	Joback Method
dvisc	0.0015236	Pa×s	526.84	Joback Method
dvisc	0.0017633	Pa×s	487.91	Joback Method
dvisc	0.0020931	Pa×s	448.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C200237&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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