Verimol K

Inchi: InChI=1S/C14H12O4/c15-11-7-4-8-12(16)13(11)14(17)18-9-10-5-2-1-3-6-10/h1-8,15-16H
InchiKey: UONCJNZKQVIGHS-UHFFFAOYSA-N
Formula: C14H12O4
SMILES: O=C(OCc1ccccc1)c1c(O)cccc1O
Mol. weight [g/mol]: 244.24
CAS: 85985-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-251.34	kJ/mol	Joback Method
hf	-458.65	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.455		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	2053.40		NIST Webbook
rinpol	2053.40		NIST Webbook
tb	810.61	K	Joback Method
tc	1066.36	K	Joback Method
tf	595.98	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.60	J/mol×K	810.61	Joback Method
cpg	562.97	J/mol×K	1023.74	Joback Method
cpg	552.13	J/mol×K	981.11	Joback Method
cpg	541.36	J/mol×K	938.49	Joback Method
cpg	530.48	J/mol×K	895.86	Joback Method
cpg	519.29	J/mol×K	853.24	Joback Method
cpg	574.07	J/mol×K	1066.36	Joback Method

dvisc	0.0000005	Pa×s	810.61	Joback Method
dvisc	0.0000008	Pa×s	774.84	Joback Method
dvisc	0.0000012	Pa×s	739.07	Joback Method
dvisc	0.0000019	Pa×s	703.30	Joback Method
dvisc	0.0000033	Pa×s	667.52	Joback Method
dvisc	0.0000061	Pa×s	631.75	Joback Method
dvisc	0.0000119	Pa×s	595.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85985757&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