Dioxadrol

Inchi: InChI=1S/C20H23NO2/c1-3-9-16(10-4-1)20(17-11-5-2-6-12-17)22-15-19(23-20)18-13-7-8
InchiKey: HGKAMARNFGKMLC-UHFFFAOYSA-N
Formula: C20H23NO2
SMILES: c1ccc(C2(c3ccccc3)OCC(C3CCCCN3)O2)cc1
Mol. weight [g/mol]: 309.40
CAS: 3666-69-1

Physical Properties

Property code	Value	Unit	Source
gf	305.61	kJ/mol	Joback Method
hf	-99.56	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.445		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	843.21	K	Joback Method
tc	1126.02	K	Joback Method
tf	564.11	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.95	J/mol×K	843.21	Joback Method
cpg	817.02	J/mol×K	890.34	Joback Method
cpg	838.91	J/mol×K	937.48	Joback Method
cpg	859.97	J/mol×K	984.61	Joback Method
cpg	880.54	J/mol×K	1031.75	Joback Method
cpg	900.97	J/mol×K	1078.88	Joback Method
cpg	921.59	J/mol×K	1126.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3666691&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
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