tetrahydro-3,4-dipiperonylfuran-2-ol

Other names: (2S,3R,4R)-3,4-bis(Benzo[d][1,3]dioxol-5-ylmethyl)tetrahydrofuran-2-ol
Inchi: InChI=1S/C20H20O6/c21-20-15(6-13-2-4-17-19(8-13)26-11-24-17)14(9-22-20)5-12-1-3-1
InchiKey: DIYWRNLYKJKHAM-UHFFFAOYSA-N
Formula: C20H20O6
SMILES: OC1OCC(Cc2ccc3c(c2)OCO3)C1Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 356.37
CAS: 18423-69-3

Physical Properties

Property code	Value	Unit	Source
gf	-105.55	kJ/mol	Joback Method
hf	-635.10	kJ/mol	Joback Method
hfus	68.27	kJ/mol	Joback Method
hvap	106.63	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.510		Crippen Method
mcvol	247.780	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	3030.30		NIST Webbook
rinpol	3030.30		NIST Webbook
tb	985.97	K	Joback Method
tc	1228.77	K	Joback Method
tf	658.53	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.25	J/mol×K	985.97	Joback Method
cpg	869.65	J/mol×K	1026.44	Joback Method
cpg	882.37	J/mol×K	1066.90	Joback Method
cpg	894.56	J/mol×K	1107.37	Joback Method
cpg	906.37	J/mol×K	1147.83	Joback Method
cpg	917.95	J/mol×K	1188.30	Joback Method

cpg	929.45	J/mol×K	1228.77	Joback Method
dvisc	0.0007663	Pa×s	658.53	Joback Method
dvisc	0.0004934	Pa×s	713.10	Joback Method
dvisc	0.0003382	Pa×s	767.68	Joback Method
dvisc	0.0002437	Pa×s	822.25	Joback Method
dvisc	0.0001830	Pa×s	876.82	Joback Method
dvisc	0.0001420	Pa×s	931.40	Joback Method
dvisc	0.0001134	Pa×s	985.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18423693&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

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