S-(-)-1,1-Diphenylprolinol

Other names:	2-Pyrrolidinemethanol, «alpha»,«alpha»-diphenyl-, (2S)-
	S -(-)- alpha , alpha -diphenyl-2-pyrrolidine methanol
Inchi:	InChI=1S/C17H19NO/c19-17(16-12-7-13-18-16,14-8-3-1-4-9-14)15-10-5-2-6-11-15/h1-6,
InchiKey:	OGCGXUGBDJGFFY-MRXNPFEDSA-N
Formula:	C17H19NO
SMILES:	OC(c1ccccc1)(c1ccccc1)C1CCCN1
Mol. weight [g/mol]:	253.34
CAS:	112068-01-6

Physical Properties

Property code	Value	Unit	Source
gf	307.36	kJ/mol	Joback Method
hf	16.16	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.675		Crippen Method
mcvol	207.860	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	794.50	K	Joback Method
tc	1043.81	K	Joback Method
tf	513.36	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.37	J/mol×K	794.50	Joback Method
cpg	642.51	J/mol×K	836.05	Joback Method
cpg	657.26	J/mol×K	877.60	Joback Method
cpg	670.76	J/mol×K	919.15	Joback Method
cpg	683.15	J/mol×K	960.70	Joback Method
cpg	694.58	J/mol×K	1002.25	Joback Method
cpg	705.18	J/mol×K	1043.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112068016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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