«alpha»,«alpha»-Diphenyl-2-piperidinepropanol

Inchi: InChI=1S/C20H25NO/c22-20(17-9-3-1-4-10-17,18-11-5-2-6-12-18)15-14-19-13-7-8-16-21
InchiKey: IUNCBCMYQPVNHW-UHFFFAOYSA-N
Formula: C20H25NO
SMILES: OC(CCC1CCCCN1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 295.42

Physical Properties

Property code	Value	Unit	Source
gf	320.52	kJ/mol	Joback Method
hf	-51.92	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	87.24	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.845		Crippen Method
mcvol	250.130	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	867.41	K	Joback Method
tc	1110.04	K	Joback Method
tf	543.65	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.71	J/mol×K	867.41	Joback Method
cpg	817.45	J/mol×K	907.85	Joback Method
cpg	832.78	J/mol×K	948.29	Joback Method
cpg	846.83	J/mol×K	988.72	Joback Method
cpg	859.72	J/mol×K	1029.16	Joback Method
cpg	871.59	J/mol×K	1069.60	Joback Method
cpg	882.58	J/mol×K	1110.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38886&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
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