Benzeneethanol, «alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha

Other names: «alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-phenylphenethyl alcohol
Propoxyphene M (des-Ac)

Inchi: InChI=1S/C19H25NO/c1-16(15-20(2)3)19(21,18-12-8-5-9-13-18)14-17-10-6-4-7-11-17/h4

InchiKey: INTCGJHAECYOBW-UHFFFAOYSA-N

Formula: C19H25NO

SMILES: CC(CN(C)C)C(O)(Cc1ccccc1)c1ccccc1

Mol. weight [g/mol]: 283.41

CAS: 126-04-5

Physical Properties

Property code	Value	Unit	Source
gf	308.28	kJ/mol	Joback Method
hf	-61.16	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.315		Crippen Method
mcvol	246.900	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	788.43	K	Joback Method
tc	1004.08	K	Joback Method
tf	437.44	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.59	J/mol×K	788.43	Joback Method
cpg	756.72	J/mol×K	824.37	Joback Method
cpg	771.72	J/mol×K	860.31	Joback Method
cpg	785.68	J/mol×K	896.25	Joback Method

cpg	798.73	J/mol×K	932.19	Joback Method
cpg	810.96	J/mol×K	968.14	Joback Method
cpg	822.49	J/mol×K	1004.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126045&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