Benzenemethanol, «alpha»-[1-(ethylmethylamino)ethyl]-, [R-(R*,S*)]-

Other names:	Etafedrine
	Benzenemethanol, «alpha»-[(1S)-1-(ethylmethylamino)ethyl]-, («alpha»R)-
	Etaphedrine
	(-)-Etafedrine
	[R-(R*,S*)]-«alpha»-[1-(ethylmethylamino)ethyl]benzyl alcohol
Inchi:	InChI=1S/C12H19NO/c1-4-13(3)10(2)12(14)11-8-6-5-7-9-11/h5-10,12,14H,4H2,1-3H3/t1
InchiKey:	IRVLBORJKFZWMI-JQWIXIFHSA-N
Formula:	C12H19NO
SMILES:	CCN(C)C(C)C(O)c1ccccc1
Mol. weight [g/mol]:	193.29
CAS:	48141-64-6

Physical Properties

Property code	Value	Unit	Source
gf	131.65	kJ/mol	Joback Method
hf	-149.74	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.060		Crippen Method
mcvol	172.030	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2093.00		NIST Webbook
tb	604.38	K	Joback Method
tc	797.18	K	Joback Method
tf	314.71	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.67	J/mol×K	604.38	Joback Method
cpg	459.61	J/mol×K	636.51	Joback Method
cpg	473.68	J/mol×K	668.65	Joback Method
cpg	486.91	J/mol×K	700.78	Joback Method
cpg	499.36	J/mol×K	732.91	Joback Method
cpg	511.06	J/mol×K	765.05	Joback Method
cpg	522.05	J/mol×K	797.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C48141646&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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