Etilefrine

Other names:	Benzenemethanol, «alpha»-[(ethylamino)methyl]-3-hydroxy-
	Benzyl alcohol, «alpha»-((ethylamino)methyl)-m-hydroxy-
	Effortil
	Ethyladrianol
	«alpha»-((Ethylamino)methyl)-m-hydroxybenzyl alcohol
	Ethyl noradrianol
	N-Ethylnorphenylephrine
	m-Hydroxyphenylethanolethylamine
	1-(3'-Hydroxyphenyl)-2-ethylaminoethanol
	Ethylphenylephrine
	Etiladrianol
	Etilefrin
	(.+/-.)-Etilefrin
	(.+/-.)-Etilefrine
	1-(3-Hydroxyphenyl)-2-(ethylamino)ethanol
	Racemic etilefrine
	S 40032
	S 40032-7
Inchi:	InChI=1S/C10H15NO2/c1-2-11-7-10(13)8-4-3-5-9(12)6-8/h3-6,10-13H,2,7H2,1H3
InchiKey:	SQVIAVUSQAWMKL-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CCNCC(O)c1cccc(O)c1
Mol. weight [g/mol]:	181.23
CAS:	709-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-58.76	kJ/mol	Joback Method
hf	-294.55	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	75.87	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.035		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook

tb	677.41	K	Joback Method
tc	884.24	K	Joback Method
tf	439.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.00	J/mol×K	677.41	Joback Method
cpg	421.16	J/mol×K	711.88	Joback Method
cpg	431.65	J/mol×K	746.35	Joback Method
cpg	441.55	J/mol×K	780.83	Joback Method
cpg	450.93	J/mol×K	815.30	Joback Method
cpg	459.86	J/mol×K	849.77	Joback Method
cpg	468.40	J/mol×K	884.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C709557&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume