1H-Imidazole, 2-[[4-(1,1-dimethylethyl)-2,6-dimethylphenyl]meth

Other names: 2-Imidazoline, 2-(4-tert-butyl-2,6-dimethylbenzyl)-
Ba-11391
Otriven
Otrivin
Otrivine
Otrix
Xylometazoline
Xylomethazoline
2-(4-tert-Butyl-2,6-dimethylbenzyl)-2-imidazoline
2-[[4-(1,1-Dimethylethyl)-2,6-dimethylphenyl]methyl]-4,5-dihydro-1H-imidazole

Inchi: InChI=1S/C16H24N2/c1-11-8-13(16(3,4)5)9-12(2)14(11)10-15-17-6-7-18-15/h8-9H,6-7,1

InchiKey: HUCJFAOMUPXHDK-UHFFFAOYSA-N

Formula: C16H24N2

SMILES: Cc1cc(C(C)(C)C)cc(C)c1CC1=NCCN1

Mol. weight [g/mol]: 244.38

CAS: 526-36-3

Physical Properties

Property code	Value	Unit	Source
gf	439.28	kJ/mol	Joback Method
hf	55.71	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
ie	8.49	eV	NIST Webbook
log10ws	-4.12		Crippen Method
logp	3.145		Crippen Method
mcvol	217.340	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2130.00		NIST Webbook
tb	730.21	K	Joback Method
tc	972.63	K	Joback Method
tf	541.47	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.30	J/mol×K	730.21	Joback Method
cpg	660.21	J/mol×K	770.61	Joback Method
cpg	678.63	J/mol×K	811.02	Joback Method
cpg	695.61	J/mol×K	851.42	Joback Method
cpg	711.23	J/mol×K	891.82	Joback Method
cpg	725.53	J/mol×K	932.23	Joback Method
cpg	738.59	J/mol×K	972.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C526363&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
ie:	Ionization energy
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