

threo-trans-Bejarol (5,9-Epoxynerolidol)

Other names:	trans-Bejarol
Inchi:	InChI=1S/C15H24O2/c1-6-15(5,16)10-14-9-12(4)8-13(17-14)7-11(2)3/h6-7,9,13-14,16H,
InchiKey:	NNCJOVBGLCRHAN-SNTRVMSOSA-N
Formula:	C15H24O2
SMILES:	<chem>C=CC(C)(O)CC1C=C(C)CC(C=C(C)C)O1</chem>
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	51.90	kJ/mol	Joback Method
hf	-332.76	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.383		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1557.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	678.24	K	Joback Method
tc	878.18	K	Joback Method
tf	344.24	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.07	J/mol×K	678.24	Joback Method
cpg	619.22	J/mol×K	711.56	Joback Method
cpg	635.33	J/mol×K	744.89	Joback Method

cpg	650.47	J/mol×K	778.21	Joback Method
cpg	664.70	J/mol×K	811.53	Joback Method
cpg	678.08	J/mol×K	844.85	Joback Method
cpg	690.67	J/mol×K	878.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232723&Units=SI

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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