anastreptene

Other names: (+)-Anastreptene
Inchi: InChI=1S/C15H22/c1-9-5-6-11-14(4)8-7-10-12(13(10,2)3)15(9,11)14/h5,10-12H,6-8H2,1-
InchiKey: SYNYVXGDEQOMCB-SEOXFTARSA-N
Formula: C15H22
SMILES: CC1=CCC2C3(C)CCC4C(C4(C)C)C123
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	318.96	kJ/mol	Joback Method
hf	-4.22	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	45.35	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.025		Crippen Method
mcvol	174.470	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1403.60		NIST Webbook
rinpol	1403.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook

ripol	1569.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1579.00		NIST Webbook
tb	560.81	K	Joback Method
tc	788.13	K	Joback Method
tf	410.59	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.78	J/mol×K	560.81	Joback Method
cpg	505.53	J/mol×K	598.70	Joback Method
cpg	524.57	J/mol×K	636.58	Joback Method
cpg	542.38	J/mol×K	674.47	Joback Method
cpg	559.40	J/mol×K	712.36	Joback Method
cpg	576.11	J/mol×K	750.24	Joback Method
cpg	592.97	J/mol×K	788.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R141830&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