Trinoranastreptene

Other names: (+)-Trisnoranastreptene
Inchi: InChI=1S/C12H16/c1-9-5-6-10-11(2)7-3-4-8-12(9,10)11/h4-5,8,10H,3,6-7H2,1-2H3
InchiKey: GOAGZWVCKOCSLC-UHFFFAOYSA-N
Formula: C12H16
SMILES: CC1=CCC2C3(C)CCC=CC123
Mol. weight [g/mol]: 160.26

Physical Properties

Property code	Value	Unit	Source
gf	259.62	kJ/mol	Joback Method
hf	55.80	kJ/mol	Joback Method
hfus	8.60	kJ/mol	Joback Method
hvap	41.16	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.309		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1189.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1189.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1455.00		NIST Webbook
tb	502.23	K	Joback Method
tc	734.55	K	Joback Method
tf	337.14	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.19	J/mol×K	502.23	Joback Method
cpg	354.05	J/mol×K	540.95	Joback Method
cpg	371.03	J/mol×K	579.67	Joback Method

cpg	386.47	J/mol×K	618.39	Joback Method
cpg	400.72	J/mol×K	657.11	Joback Method
cpg	414.10	J/mol×K	695.83	Joback Method
cpg	426.97	J/mol×K	734.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240145&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
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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