8a-Isopropyl-3-methyl-1,2,4,5,8,8a-hexahydroazul

Inchi: InChI=1S/C15H22O/c1-11(2)15-8-6-12(3)14(15)5-4-13(10-16)7-9-15/h7,10-11H,4-6,8-9H
InchiKey: MWDZEHCTRAXXDY-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC1=C2CCC(C=O)=CCC2(C(C)C)CC1
Mol. weight [g/mol]: 218.33
CAS: 311351-24-3

Physical Properties

Property code	Value	Unit	Source
gf	79.81	kJ/mol	Joback Method
hf	-206.10	kJ/mol	Joback Method
hfus	15.15	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1693.60		NIST Webbook
rinpol	1693.60		NIST Webbook
tb	639.55	K	Joback Method
tc	866.52	K	Joback Method
tf	374.83	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.33	J/mol×K	639.55	Joback Method
cpg	544.47	J/mol×K	677.38	Joback Method
cpg	562.52	J/mol×K	715.21	Joback Method
cpg	579.64	J/mol×K	753.03	Joback Method
cpg	596.00	J/mol×K	790.86	Joback Method
cpg	611.75	J/mol×K	828.69	Joback Method
cpg	627.07	J/mol×K	866.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C311351243&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