

(3S,3aS,6R)-7,7,8-Trimethyl-2,3,4,5,6,7-hexahydroisoindolizino[1,2-b]pyridine-3-carboxylic acid

Other names:	1H-3a,6-Methanoazulene-3-carboxylic acid, 2,3,4,5,6,7-hexahydro-7,7,8-trimethyl- (3S,3aS,6R)- 1H-3a,6-Methanoazulene-3-carboxylic acid, 2,3,4,5,6,7-hexahydro-7,7,8-trimethyl- [3S-(3«alpha»,3a«alpha»,6«alpha»)]- 1H-3a«alpha»,6-Methanoazulene-3-carboxylic acid, 2,3«beta»,4,5,6«beta»,7-hexahydro-7,7,8-trimethyl- isokhusenic acid Isozizanoic acid
Inchi:	InChI=1S/C15H22O2/c1-9-11-4-5-12(13(16)17)15(11)7-6-10(8-15)14(9,2)3/h10,12H,4-8H
InchiKey:	DHPMFKAJSXGYDJ-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CC1=C2CCC(C(=O)O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	234.33
CAS:	16202-79-2

Physical Properties

Property code	Value	Unit	Source
gf	-40.26	kJ/mol	Joback Method
hf	-366.68	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.624		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1786.00		NIST Webbook
tb	722.34	K	Joback Method
tc	938.29	K	Joback Method
tf	485.70	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.90	J/mol×K	722.34	Joback Method
cpg	609.76	J/mol×K	758.33	Joback Method
cpg	626.31	J/mol×K	794.32	Joback Method

cpg	642.80	J/mol×K	830.31	Joback Method
cpg	659.49	J/mol×K	866.31	Joback Method
cpg	676.65	J/mol×K	902.30	Joback Method
cpg	694.52	J/mol×K	938.29	Joback Method

Sources

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=C16202792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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