

15-nor-Prezizaan-7-one

Inchi:	InChI=1S/C14H22O/c1-9-4-5-11-13(2,3)12(15)10-6-7-14(9,11)8-10/h9-11H,4-8H2,1-3H3
InchiKey:	JUNOMGCJVMTXEV-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC1CCC2C(C)(C)C(=O)C3CCC12C3
Mol. weight [g/mol]:	206.32
CAS:	114299-44-4

Physical Properties

Property code	Value	Unit	Source
gf	76.06	kJ/mol	Joback Method
hf	-274.11	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.428		Crippen Method
mvol	177.110	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1581.10		NIST Webbook
rinpol	1581.10		NIST Webbook
tb	607.44	K	Joback Method
tc	847.85	K	Joback Method
tf	401.86	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.23	J/molxK	607.44	Joback Method
cpg	534.02	J/molxK	647.51	Joback Method
cpg	555.46	J/molxK	687.58	Joback Method
cpg	575.85	J/molxK	727.65	Joback Method
cpg	595.52	J/molxK	767.72	Joback Method
cpg	614.78	J/molxK	807.79	Joback Method
cpg	633.95	J/molxK	847.85	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=C114299444&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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