

Tricyclo[7.3.0.0(3,8)]dodec-1(9)-en-12-one, 2,2-dicyano, cis-

Other names:	Tricyclo[7.3.0.0(3,8)]dodec-1(9)-en-12-one,2,2-dicyano, (Z)
Inchi:	InChI=1S/C14H14N2O/c15-7-14(8-16)11-4-2-1-3-9(11)10-5-6-12(17)13(10)14/h9,11H,1-
InchiKey:	YTDGQCZUJWOVNZ-UHFFFAOYSA-N
Formula:	C14H14N2O
SMILES:	N#CC1(C#N)C2=C(CCC2=O)C2CCCCC21
Mol. weight [g/mol]:	226.27

Physical Properties

Property code	Value	Unit	Source
gf	361.93	kJ/mol	Joback Method
hf	109.77	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.499		Crippen Method
mvol	175.570	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	834.09	K	Joback Method
tc	1097.05	K	Joback Method
tf	538.70	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.35	J/molxK	834.09	Joback Method
cpg	564.21	J/molxK	877.92	Joback Method
cpg	579.88	J/molxK	921.74	Joback Method
cpg	595.62	J/molxK	965.57	Joback Method
cpg	611.67	J/molxK	1009.39	Joback Method
cpg	628.28	J/molxK	1053.22	Joback Method
cpg	645.70	J/molxK	1097.05	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=U160538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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