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

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]: 226.28

Physical Properties

Property code	Value	Unit	Source
hfus	16.79	kJ/mol	Joback Method
logp	2.499		Crippen Method
mcvol	175.570	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.35	J/mol×K	834.09	Joback Method
cpg	564.21	J/mol×K	877.92	Joback Method
cpg	579.88	J/mol×K	921.74	Joback Method
cpg	595.62	J/mol×K	965.57	Joback Method
cpg	611.67	J/mol×K	1009.39	Joback Method
cpg	628.28	J/mol×K	1053.22	Joback Method
cpg	645.70	J/mol×K	1097.05	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U160538&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices