

2,2':6',2''-TERPYRIDINE

Other names:	«alpha»,«alpha»',«alpha»"-Terpyridine 2,2':6',2''-Terpyridine «alpha»,«alpha»',«alpha»"-Tripyridyl Ba 2799 Tripyridine 2,2',2''-Terpyridine 2,2',2''-Terpyridyl 2,2',2''-Tripyridine 2,2',2''-Tripyridyl 2,6-Bis(2-pyridyl)pyridine NSC 36755 NSC 3905 2,2':6',2''-Terpyridine
Inchi:	InChI=1S/C15H11N3/c1-3-10-16-12(6-1)14-8-5-9-15(18-14)13-7-2-4-11-17-13/h1-11H
InchiKey:	DRGAZIDRYFYHIJ-UHFFFAOYSA-N
Formula:	C15H11N3
SMILES:	c1ccc(-c2cccc(-c3cccn3)n2)nc1
Mol. weight [g/mol]:	233.27

Physical Properties

Property code	Value	Unit	Source
af	0.5167		Cheméo Relay (1.0)
chs	-7772.30 ± 3.30	kJ/mol	NIST Webbook
gf	428.38	kJ/mol	Cheméo Relay (1.0, beta)
hf	394.60 ± 4.60	kJ/mol	NIST Webbook
hfs	297.50 ± 3.50	kJ/mol	NIST Webbook
hsub	97.10	kJ/mol	NIST Webbook
hsub	97.10 ± 1.10	kJ/mol	NIST Webbook
hvap	107.60	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-3.06		Cheméo Relay (1.0)
logp	3.206		Crippen Method
mcvol	180.870	ml/mol	McGowan Method
pc	4178.02	kPa	Cheméo Relay (1.0, beta)
tb	657.86	K	Cheméo Relay (1.0)
tc	953.44	K	Cheméo Relay (1.0)
tf	399.96	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1148794&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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