2-ISOPROPYL-4,5-DIMETHYLTHIAZOLE

Other names: 4,5-Dimethyl-2-isopropyl-thiazole
Thiazole, 4,5-dimethyl-2-isopropyl
Inchi: InChI=1S/C8H13NS/c1-5(2)8-9-6(3)7(4)10-8/h5H,1-4H3
InchiKey: GDYKEHYOOVICQZ-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: Cc1nc(C(C)C)sc1C
Mol. weight [g/mol]: 155.27

Physical Properties

Property code	Value	Unit	Source
ie	8.35	eV	Cheméo Relay (1.0)
logp	2.883		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1097.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1433.00		NIST Webbook
tf	267.86	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53498309&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
Cheméo Relay (1.0):

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point