3,4-dimethylquinoline

Inchi: InChI=1S/C11H11N/c1-8-7-12-11-6-4-3-5-10(11)9(8)2/h3-7H,1-2H3
InchiKey: QOSYOGXDDHFINM-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1cnc2ccccc2c1C
Mol. weight [g/mol]: 157.22
CAS: 2436-92-2

Physical Properties

Property code	Value	Unit	Source
af	0.4266		Cheméo Relay (1.0)
hf	143.31	kJ/mol	Cheméo Relay (1.0)
hvap	68.13	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-2.27		Cheméo Relay (1.0)
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
pc	3843.84	kPa	Cheméo Relay (1.0, beta)
tb	549.48	K	Cheméo Relay (1.0)
tc	811.79	K	Cheméo Relay (1.0)
tf	311.56	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59519e+01
Coeff. B	-5.01000e+03
Coeff. C	-9.79840e+01
Temperature range (K), min.	417.82
Temperature range (K), max.	568.83

Sources

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):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
hf:	Enthalpy of formation 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume