2-Ethyl-4-methylpyridine

Inchi: InChI=1S/C8H11N/c1-3-8-6-7(2)4-5-9-8/h4-6H,3H2,1-2H3
InchiKey: WFGFGSWFQKXOAE-UHFFFAOYSA-N
Formula: C8H11N
SMILES: CCc1cc(C)ccn1
Mol. weight [g/mol]: 121.18
CAS: 2150-18-7

Physical Properties

Property code	Value	Unit	Source
af	0.3782		Cheméo Relay (1.0)
hf	37.11	kJ/mol	Cheméo Relay (1.0)
hvap	48.44	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-0.41		Cheméo Relay (1.0)
logp	1.952		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3545.81	kPa	Cheméo Relay (1.0, beta)
rinpol	1027.00		NIST Webbook
rinpol	1013.00		NIST Webbook
tb	447.09	K	Cheméo Relay (1.0)
tc	652.73	K	Cheméo Relay (1.0)
tf	226.42	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41568e+01
Coeff. B	-3.70672e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	332.72
Temperature range (K), max.	484.52

Sources

Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2150187&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point