3-ethyl-2,5-dimethyl-5,6-dihydropyrazine

Inchi: InChI=1S/C8H14N2/c1-4-8-7(3)9-5-6(2)10-8/h6H,4-5H2,1-3H3
InchiKey: QLBAZJOHRSXXKD-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: CCC1=NC(C)CN=C1C
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	315.15	kJ/mol	Joback Method
hf	80.43	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.700		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1031.00		NIST Webbook
tb	517.67	K	Joback Method
tc	748.25	K	Joback Method
tf	356.94	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.16	J/mol×K	517.67	Joback Method
cpg	321.06	J/mol×K	556.10	Joback Method
cpg	338.07	J/mol×K	594.53	Joback Method
cpg	354.18	J/mol×K	632.96	Joback Method
cpg	369.36	J/mol×K	671.39	Joback Method
cpg	383.58	J/mol×K	709.82	Joback Method
cpg	396.82	J/mol×K	748.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume