3-tert-BUTYL-2-PYRAZOLIN-5-ONE

Inchi: InChI=1S/C7H12N2O/c1-7(2,3)5-4-6(10)9-8-5/h4H2,1-3H3,(H,9,10)
InchiKey: VDNOHRWEOSDGQX-UHFFFAOYSA-N
Formula: C7H12N2O
SMILES: CC(C)(C)C1=NNC(=O)C1
Mol. weight [g/mol]: 140.19

Physical Properties

Property code	Value	Unit	Source
hfus	14.41	kJ/mol	Joback Method
logp	0.908		Crippen Method
mcvol	115.860	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.33	J/mol×K	550.49	Joback Method
cpg	304.39	J/mol×K	592.15	Joback Method
cpg	319.49	J/mol×K	633.82	Joback Method
cpg	333.60	J/mol×K	675.48	Joback Method
cpg	346.73	J/mol×K	717.14	Joback Method
cpg	358.86	J/mol×K	758.81	Joback Method
cpg	369.99	J/mol×K	800.47	Joback Method

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29211685&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume