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

Other names: 2-butyl-3,5-dimethyl-5,6-dihydropyrazine
Inchi: InChI=1S/C10H18N2/c1-4-5-6-10-9(3)12-8(2)7-11-10/h8H,4-7H2,1-3H3
InchiKey: UCGBLZSNPDKNEM-UHFFFAOYSA-N
Formula: C10H18N2
SMILES: CCCCC1=NCC(C)N=C1C
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	331.99	kJ/mol	Joback Method
hf	39.15	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	52.61	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.481		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	563.43	K	Joback Method
tc	785.66	K	Joback Method
tf	379.48	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.33	J/mol×K	563.43	Joback Method
cpg	418.82	J/mol×K	600.47	Joback Method
cpg	437.28	J/mol×K	637.51	Joback Method
cpg	454.71	J/mol×K	674.55	Joback Method
cpg	471.08	J/mol×K	711.59	Joback Method
cpg	486.38	J/mol×K	748.62	Joback Method
cpg	500.60	J/mol×K	785.66	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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