Azetidine, 3-methyl-3-phenyl-

Other names: L 1834
3-Methyl-3-phenylazetidine
Inchi: InChI=1S/C10H13N/c1-10(7-11-8-10)9-5-3-2-4-6-9/h2-6,11H,7-8H2,1H3
InchiKey: YOLLUMURPUEOJW-UHFFFAOYSA-N
Formula: C10H13N
SMILES: CC1(c2ccccc2)CNC1
Mol. weight [g/mol]: 147.22
CAS: 5961-33-1

Physical Properties

Property code	Value	Unit	Source
gf	276.60	kJ/mol	Joback Method
hf	106.49	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	45.82	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.548		Crippen Method
mcvol	127.120	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	514.68	K	Joback Method
tc	761.92	K	Joback Method
tf	372.23	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.47	J/mol×K	514.68	Joback Method
cpg	301.59	J/mol×K	555.89	Joback Method
cpg	317.29	J/mol×K	597.09	Joback Method
cpg	331.76	J/mol×K	638.30	Joback Method
cpg	345.22	J/mol×K	679.51	Joback Method
cpg	357.85	J/mol×K	720.71	Joback Method
cpg	369.84	J/mol×K	761.92	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C5961331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume