2-Benzyl-4,4,6-trimethyl-5,6-dihydro-1,3(4H)oxazir

Other names: 5,6-Dihydro-2-benzyl-4,4,6-trimethyl-(4H)-1,3-oxazine
4H-1,3-Oxazine, 5,6-dihydro-4,4,6-trimethyl-2-(phenylmethyl)-
2-benzyl-5,6-dihydro-4,4,6-trimethyl-4H-1,3-oxazine
Inchi: InChI=1S/C14H19NO/c1-11-10-14(2,3)15-13(16-11)9-12-7-5-4-6-8-12/h4-8,11H,9-10H2,
InchiKey: KDQDSZHGNOYQGK-UHFFFAOYSA-N
Formula: C14H19NO
SMILES: CC1CC(C)(C)N=C(Cc2ccccc2)O1
Mol. weight [g/mol]: 217.31
CAS: 26939-22-0

Physical Properties

Property code	Value	Unit	Source
gf	241.65	kJ/mol	Joback Method
hf	-61.26	kJ/mol	Joback Method
hfus	26.62	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.215		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
tb	646.31	K	Joback Method
tc	894.48	K	Joback Method
tf	412.39	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.53	J/mol×K	646.31	Joback Method
cpg	536.47	J/mol×K	687.67	Joback Method
cpg	556.05	J/mol×K	729.03	Joback Method
cpg	574.43	J/mol×K	770.39	Joback Method
cpg	591.78	J/mol×K	811.75	Joback Method
cpg	608.25	J/mol×K	853.11	Joback Method

cpg	623.99	J/mol×K	894.48	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=C26939220&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