

Terpinen-4-ol, carbamate

Inchi:	InChI=1S/C11H19NO2/c1-8(2)11(14-10(12)13)6-4-9(3)5-7-11/h4,8H,5-7H2,1-3H3,(H2,12)
InchiKey:	HGIZGFXYKVVJOOT-UHFFFAOYSA-N
Formula:	C11H19NO2
SMILES:	CC1=CCC(OC(N)=O)(C(C)C)CC1
Mol. weight [g/mol]:	197.27

Physical Properties

Property code	Value	Unit	Source
gf	-88.88	kJ/mol	Joback Method
hf	-370.79	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.607		Crippen Method
mvol	168.110	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	623.39	K	Joback Method
tc	849.46	K	Joback Method
tf	398.71	K	Joback Method
vc	0.616	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.50	J/mol×K	623.39	Joback Method
cpg	466.24	J/mol×K	661.07	Joback Method
cpg	482.05	J/mol×K	698.75	Joback Method
cpg	497.06	J/mol×K	736.43	Joback Method
cpg	511.37	J/mol×K	774.11	Joback Method
cpg	525.10	J/mol×K	811.79	Joback Method
cpg	538.36	J/mol×K	849.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R579478&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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