

Isopulegol, carbamate

Inchi:	InChI=1S/C11H19NO2/c1-7(2)9-5-4-8(3)6-10(9)14-11(12)13/h8-10H,1,4-6H2,2-3H3,(H2,
InchiKey:	RZCGKLPOLDEBS-AEJSXWLSSA-N
Formula:	C11H19NO2
SMILES:	C=C(C)C1CCC(C)CC1OC(N)=O
Mol. weight [g/mol]:	197.27

Physical Properties

Property code	Value	Unit	Source
gf	-37.41	kJ/mol	Joback Method
hf	-352.10	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.463		Crippen Method
mvol	168.110	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1456.00		NIST Webbook
tb	606.67	K	Joback Method
tc	825.13	K	Joback Method
tf	352.33	K	Joback Method
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.82	J/mol×K	606.67	Joback Method
cpg	473.39	J/mol×K	643.08	Joback Method
cpg	490.88	J/mol×K	679.49	Joback Method
cpg	507.30	J/mol×K	715.90	Joback Method
cpg	522.66	J/mol×K	752.31	Joback Method
cpg	536.97	J/mol×K	788.72	Joback Method
cpg	550.25	J/mol×K	825.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mccvol:	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

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