(1R)-(+)-pulegone

Inchi: InChI=1S/C11H20O/c1-5-7-8-10(9(3)4)11(12)6-2/h5-8H2,1-4H3
InchiKey: NHPCTOQWRLAEGD-UHFFFAOYSA-N
Formula: C11H20O
SMILES: CCCCC(C(=O)CC)=C(C)C
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
gf	-24.06	kJ/mol	Joback Method
hf	-285.31	kJ/mol	Joback Method
hfus	23.43	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.492		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1241.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	508.87	K	Joback Method
tc	694.01	K	Joback Method
tf	230.66	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.72	J/mol×K	508.87	Joback Method
cpg	386.10	J/mol×K	539.73	Joback Method
cpg	400.75	J/mol×K	570.58	Joback Method
cpg	414.70	J/mol×K	601.44	Joback Method
cpg	427.98	J/mol×K	632.30	Joback Method
cpg	440.62	J/mol×K	663.16	Joback Method
cpg	452.64	J/mol×K	694.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R283815&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume