Methyl pulegenate

Inchi: InChI=1S/C11H18O2/c1-7(2)9-6-5-8(3)10(9)11(12)13-4/h8,10H,5-6H2,1-4H3/t8-,10-/m0/s
InchiKey: DVRISWLNCBSESY-WPRPVWTQSA-N
Formula: C11H18O2
SMILES: COC(=O)C1C(=C(C)C)CCC1C
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-126.43	kJ/mol	Joback Method
hf	-408.79	kJ/mol	Joback Method
hfus	21.05	kJ/mol	Joback Method
hvap	50.05	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.542		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
ripol	1499.00		NIST Webbook
tb	544.50	K	Joback Method
tc	749.73	K	Joback Method
tf	288.95	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.78	J/mol×K	544.50	Joback Method
cpg	403.01	J/mol×K	578.70	Joback Method
cpg	419.37	J/mol×K	612.91	Joback Method
cpg	434.90	J/mol×K	647.11	Joback Method
cpg	449.61	J/mol×K	681.32	Joback Method
cpg	463.50	J/mol×K	715.52	Joback Method
cpg	476.61	J/mol×K	749.73	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=R621113&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume