

(E)-pulegol

Other names:	trans-pulegol
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h8,10-11H,4-6H2,1-3H3/t8-,10+/m1/s1
InchiKey:	JGVWYJDASSSGEK-SCZZXKLOSA-N
Formula:	C10H18O
SMILES:	CC(C)=C1CCC(C)CC1O
Mol. weight [g/mol]:	154.25
CAS:	22472-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-49.85	kJ/mol	Joback Method
hf	-301.74	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.504		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	541.78	K	Joback Method
tc	736.93	K	Joback Method
tf	262.82	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.40	J/mol×K	541.78	Joback Method
cpg	367.35	J/mol×K	574.31	Joback Method
cpg	382.51	J/mol×K	606.83	Joback Method
cpg	396.91	J/mol×K	639.36	Joback Method
cpg	410.57	J/mol×K	671.88	Joback Method

cpg	423.50	J/mol×K	704.41	Joback Method
cpg	435.72	J/mol×K	736.93	Joback Method

Sources

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=C22472793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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