apopinene

Inchi: InChI=1S/C9H14/c1-9(2)7-4-3-5-8(9)6-7/h3-4,7-8H,5-6H2,1-2H3
InchiKey: SUEFRHDDZDWKFN-UHFFFAOYSA-N
Formula: C9H14
SMILES: CC1(C)C2C=CCC1C2
Mol. weight [g/mol]: 122.21
CAS: 32863-61-9

Physical Properties

Property code	Value	Unit	Source
gf	151.06	kJ/mol	Joback Method
hf	-36.97	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	34.46	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.609		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	924.00		NIST Webbook
ripol	1060.00		NIST Webbook
tb	417.80	K	Joback Method
tc	628.03	K	Joback Method
tf	243.97	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.34	J/mol×K	417.80	Joback Method
cpg	247.34	J/mol×K	452.84	Joback Method
cpg	263.89	J/mol×K	487.88	Joback Method
cpg	279.13	J/mol×K	522.92	Joback Method

cpg	293.18	J/mol×K	557.96	Joback Method
cpg	306.20	J/mol×K	592.99	Joback Method
cpg	318.32	J/mol×K	628.03	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=C32863619&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
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