

4-Ethylcamphor

Inchi:	InChI=1S/C12H20O/c1-5-12-7-6-11(4,9(13)8-12)10(12,2)3/h5-8H2,1-4H3
InchiKey:	CKBXFJIWHMQXQW-UHFFFAOYSA-N
Formula:	C12H20O
SMILES:	CCC12CCC(C)(C(=O)C1)C2(C)C
Mol. weight [g/mol]:	180.29
CAS:	90547-83-4

Physical Properties

Property code	Value	Unit	Source
affp	865.10	kJ/mol	NIST Webbook
basg	833.30	kJ/mol	NIST Webbook
gf	12.79	kJ/mol	Joback Method
hf	-263.89	kJ/mol	Joback Method
hfus	2.69	kJ/mol	Joback Method
hvap	42.79	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.182		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	555.58	K	Joback Method
tc	789.43	K	Joback Method
tf	393.04	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.97	J/mol×K	555.58	Joback Method
cpg	438.16	J/mol×K	594.55	Joback Method
cpg	456.00	J/mol×K	633.53	Joback Method
cpg	472.87	J/mol×K	672.50	Joback Method
cpg	489.14	J/mol×K	711.48	Joback Method
cpg	505.18	J/mol×K	750.45	Joback Method
cpg	521.38	J/mol×K	789.43	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=C90547834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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