BICYCLO[2.2.1]HEPTAN-2-ONE, 7,7-DIMETHYL-

Other names: «alpha»-Fenchocamphone
Inchi: InChI=1S/C9H14O/c1-9(2)6-3-4-7(9)8(10)5-6/h6-7H,3-5H2,1-2H3
InchiKey: DOCLMTQMWGMALI-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1(C)C2CCC1C(=O)C2
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
hf	-204.85	kJ/mol	Cheméo Relay (1.0)
hfus	7.52	kJ/mol	Joback Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
tb	468.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.51	J/mol×K	486.46	Joback Method
cpg	296.15	J/mol×K	524.28	Joback Method
cpg	312.56	J/mol×K	562.10	Joback Method
cpg	327.88	J/mol×K	599.93	Joback Method
cpg	342.24	J/mol×K	637.75	Joback Method
cpg	355.78	J/mol×K	675.57	Joback Method
cpg	368.63	J/mol×K	713.39	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C514158&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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