

Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-

Other names:	(-)-Alcanfor (-)-Camphor Camphor, (1S,4S)-(-)- L-camphor Levo-(-)-camphor (1S)-(-)-Camphor Camphor, l-, (-)- 1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one, (1S,4S)- S-(-)-Camphor Camphore (-)-bornan-2-one
Inchi:	InChI=1S/C10H16O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7H,4-6H2,1-3H3
InchiKey:	DSSYKIVIOFKYAU-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC12CCC(CC1=O)C2(C)C
Mol. weight [g/mol]:	152.23
CAS:	464-48-2

Physical Properties

Property code	Value	Unit	Source
gf	1.44	kJ/mol	Joback Method
hf	-237.85	kJ/mol	Joback Method
hfus	3.81	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	477.20	K	NIST Webbook
tc	742.46	K	Joback Method

tf	453.20 ± 1.50	K	NIST Webbook
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	509.58	Joback Method
cpg	342.61	J/mol×K	548.39	Joback Method
cpg	359.48	J/mol×K	587.21	Joback Method
cpg	375.18	J/mol×K	626.02	Joback Method
cpg	389.96	J/mol×K	664.83	Joback Method
cpg	404.06	J/mol×K	703.65	Joback Method
cpg	417.76	J/mol×K	742.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C464482&Units=SI

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:	Non-polar retention indices
ripol:	Polar retention indices

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

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