

Bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-

Other names: 2-Chlorocamphane
Bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-
Bornane, 2-chloro-, endo-
Pinene hydrochloride
Terpene hydrochloride
Turpentine camphor
endo-2-Chloro-1,7,7-trimethylbicyclo[2.2.1]heptane
endo-2-chlorobornane

Inchi: InChI=1S/C10H17Cl/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7-8H,4-6H2,1-3H3
InchiKey: XXZAOMJCZBZKPV-UHFFFAOYSA-N
Formula: C10H17Cl
SMILES: CC1(C)C2CCC1(C)C(Cl)C2
Mol. weight [g/mol]: 172.70

Physical Properties

Property code	Value	Unit	Source
hfus	9.57	kJ/mol	Joback Method
log10ws	-4.40		Cheméo Relay (1.0)
logp	3.440		Crippen Method
mcvol	142.280	ml/mol	McGowan Method
tb	480.50	K	Cheméo Relay (1.0)
tf	404.00 ± 4.00	K	NIST Webbook
tf	400.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.18	J/mol×K	474.52	Joback Method
cpg	341.45	J/mol×K	511.36	Joback Method
cpg	359.03	J/mol×K	548.21	Joback Method
cpg	375.17	J/mol×K	585.05	Joback Method
cpg	390.11	J/mol×K	621.90	Joback Method
cpg	404.10	J/mol×K	658.74	Joback Method
cpg	417.38	J/mol×K	695.58	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C464415&Units=SI>

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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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