Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, (1«alpha»,3«alpha»,6«alpha»)-

Other names: Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, (1«beta»,3«beta»,6«beta»)-
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, (1Â«betaÂ»,3Â«betaÂ»,6Â«betaÂ»)-
Carane, trans-
trans-Carane

Inchi: InChI=1S/C10H18/c1-7-4-5-8-9(6-7)10(8,2)3/h7-9H,4-6H2,1-3H3/t7-,8-,9+/m1/s1

InchiKey: BWRHOYDPVJPXMF-HLTSFMKQSA-N

Formula: C10H18

SMILES: CC1CCC2C(C1)C2(C)C

Mol. weight [g/mol]: 138.25

CAS: 18968-23-5

Physical Properties

Property code	Value	Unit	Source
gf	121.81	kJ/mol	Joback Method
hf	-135.73	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	36.08	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	977.50		NIST Webbook
tb	436.85	K	Joback Method
tc	642.10	K	Joback Method
tf	250.24	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.02	J/mol×K	436.85	Joback Method
cpg	307.28	J/mol×K	471.06	Joback Method
cpg	326.14	J/mol×K	505.27	Joback Method
cpg	343.70	J/mol×K	539.47	Joback Method

cpg	360.10	J/mol×K	573.68	Joback Method
cpg	375.46	J/mol×K	607.89	Joback Method
cpg	389.91	J/mol×K	642.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.19911e+01
Coeff. B	-2.88103e+03
Coeff. C	-7.10880e+01
Temperature range (K), min.	317.26
Temperature range (K), max.	502.40

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18968235&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

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume