

cis-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-/m0/s1
InchiKey:	BWRHOYDPVJPXMF-YIZRAAEISA-N
Formula:	C10H18
SMILES:	CC1CCC2C(C1)C2(C)C
Mol. weight [g/mol]:	138.25
CAS:	18968-24-6

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	975.00		NIST Webbook
tb	436.85	K	Joback Method
tc	642.10	K	Joback Method
tf	250.24	K	Joback Method
vc	0.497	m ³ /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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.19705e+01
Coeff. B	-2.88773e+03
Coeff. C	-6.90810e+01
Temperature range (K), min.	316.26
Temperature range (K), max.	502.74

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492227&Units=SI
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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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