

trans-4a-Methyl-decahydronaphthalene

Other names:	trans-9-Methyldecalin 1-Methyl-trans-bicyclo[4.4.0]decane
Inchi:	InChI=1S/C11H20/c1-11-8-4-2-6-10(11)7-3-5-9-11/h10H,2-9H2,1H3/t10-,11-
InchiKey:	RAFDCSMAXTUJKJ-XYPPYZODXSA-N
Formula:	C11H20
SMILES:	CC12CCCCC1CCCC2
Mol. weight [g/mol]:	152.28
CAS:	2547-27-5

Physical Properties

Property code	Value	Unit	Source
chl	-6937.20 ± 1.70	kJ/mol	NIST Webbook
gf	109.35	kJ/mol	Joback Method
hf	-134.17	kJ/mol	Joback Method
hfl	-249.80 ± 1.80	kJ/mol	NIST Webbook
hfus	5.82	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.757		Crippen Method
mcvol	144.130	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	481.88	K	Joback Method
tc	710.30	K	Joback Method
tf	259.43	K	Joback Method
vc	0.531	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.23	J/mol×K	481.88	Joback Method
cpg	357.60	J/mol×K	519.95	Joback Method
cpg	379.26	J/mol×K	558.02	Joback Method
cpg	399.38	J/mol×K	596.09	Joback Method
cpg	418.13	J/mol×K	634.16	Joback Method

cpg	435.67	J/mol×K	672.23	Joback Method
cpg	452.17	J/mol×K	710.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2547275&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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