

TRANS-DECALIN, 2-METHYL-

Other names:	2-Methyldecalin, trans
Inchi:	InChI=1S/C11H20/c1-9-6-7-10-4-2-3-5-11(10)8-9/h9-11H,2-8H2,1H3
InchiKey:	GREARFRXIFVLGB-UHFFFAOYSA-N
Formula:	C11H20
SMILES:	CC1CCC2CCCCC2C1
Mol. weight [g/mol]:	152.28

Physical Properties

Property code	Value	Unit	Source
af	0.2857		Cheméo Relay (1.0)
gf	107.13	kJ/mol	Joback Method
hf	-169.63	kJ/mol	Cheméo Relay (1.0)
hfus	13.19	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-5.58		Cheméo Relay (1.0)
logp	3.613		Crippen Method
mcvol	144.130	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	478.30	K	Cheméo Relay (1.0)
tc	697.74	K	Cheméo Relay (1.0)
tf	233.61	K	Cheméo Relay (1.0)
vc	0.514	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.53	J/mol×K	476.97	Joback Method
cpg	356.99	J/mol×K	513.37	Joback Method
cpg	379.11	J/mol×K	549.78	Joback Method
cpg	399.91	J/mol×K	586.18	Joback Method
cpg	419.46	J/mol×K	622.58	Joback Method

cpg	437.80	J/mol×K	658.98	Joback Method
cpg	454.99	J/mol×K	695.39	Joback Method
dvisc	0.0031852	Pa×s	231.29	Joback Method
dvisc	0.0017507	Pa×s	272.24	Joback Method
dvisc	0.0011253	Pa×s	313.18	Joback Method
dvisc	0.0008011	Pa×s	354.13	Joback Method
dvisc	0.0006120	Pa×s	395.08	Joback Method
dvisc	0.0004917	Pa×s	436.02	Joback Method
dvisc	0.0004102	Pa×s	476.97	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U152473&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/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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