

«alpha»-n-Propyldecalin

Inchi:	InChI=1S/C13H24/c1-2-6-11-8-5-9-12-7-3-4-10-13(11)12/h11-13H,2-10H2,1H3
InchiKey:	HIXIFRGJVIZERN-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	CCCC1CCCC2CCCCC12
Mol. weight [g/mol]:	180.33
CAS:	91972-45-1

Physical Properties

Property code	Value	Unit	Source
gf	123.97	kJ/mol	Joback Method
hf	-211.03	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.393		Crippen Method
mcvol	172.310	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
tb	522.73	K	Joback Method
tc	734.35	K	Joback Method
tf	253.83	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.38	J/mol×K	558.00	Joback Method
cpg	433.98	J/mol×K	522.73	Joback Method
cpg	560.61	J/mol×K	734.35	Joback Method
cpg	542.63	J/mol×K	699.08	Joback Method
cpg	523.47	J/mol×K	663.81	Joback Method
cpg	503.08	J/mol×K	628.54	Joback Method
cpg	481.40	J/mol×K	593.27	Joback Method
cpl	337.20	J/mol×K	313.00	NIST Webbook
cpl	335.60	J/mol×K	311.00	NIST Webbook

dvisc	0.0003951	Pa×s	522.73	Joback Method
dvisc	0.0004821	Pa×s	477.91	Joback Method
dvisc	0.0006128	Pa×s	433.10	Joback Method
dvisc	0.0008235	Pa×s	388.28	Joback Method
dvisc	0.0011953	Pa×s	343.46	Joback Method
dvisc	0.0019401	Pa×s	298.65	Joback Method
dvisc	0.0037366	Pa×s	253.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91972451&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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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