2-Butyldecalin, cis

Inchi: InChI=1S/C14H26/c1-2-3-6-12-9-10-13-7-4-5-8-14(13)11-12/h12-14H,2-11H2,1H3/t12?,1
InchiKey: VYMIQGUNEIJWAR-KFTPUPIBSA-N
Formula: C14H26
SMILES: CCCCC1CCC2CCCCC2C1
Mol. weight [g/mol]: 194.36

Physical Properties

Property code	Value	Unit	Source
gf	132.39	kJ/mol	Joback Method
hf	-231.67	kJ/mol	Joback Method
hfus	20.96	kJ/mol	Joback Method
hvap	46.96	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.783		Crippen Method
mcvol	186.400	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	545.61	K	Joback Method
tc	753.90	K	Joback Method
tf	265.10	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.63	J/mol×K	545.61	Joback Method
cpg	511.33	J/mol×K	580.32	Joback Method
cpg	534.64	J/mol×K	615.04	Joback Method
cpg	556.61	J/mol×K	649.75	Joback Method
cpg	577.29	J/mol×K	684.47	Joback Method
cpg	596.73	J/mol×K	719.18	Joback Method
cpg	614.98	J/mol×K	753.90	Joback Method
dvisc	0.0039102	Pa×s	265.10	Joback Method

dvisc	0.0019806	Pa×s	311.85	Joback Method
dvisc	0.0011979	Pa×s	358.60	Joback Method
dvisc	0.0008136	Pa×s	405.36	Joback Method
dvisc	0.0005986	Pa×s	452.11	Joback Method
dvisc	0.0004665	Pa×s	498.86	Joback Method
dvisc	0.0003794	Pa×s	545.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R578217&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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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