1,1'-Bicyclohexyl, 2-butyl-

Inchi: InChI=1S/C16H30/c1-2-3-9-14-12-7-8-13-16(14)15-10-5-4-6-11-15/h14-16H,2-13H2,1H3
InchiKey: NUHOLGQIGHXQAE-UHFFFAOYSA-N
Formula: C16H30
SMILES: CCCCC1CCCCC1C1CCCCC1
Mol. weight [g/mol]: 222.41
CAS: 54889-99-5

Physical Properties

Property code	Value	Unit	Source
gf	125.03	kJ/mol	Joback Method
hf	-285.27	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.563		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
tb	567.30 ± 0.40	K	NIST Webbook
tb	569.71 ± 0.40	K	NIST Webbook
tc	815.62	K	Joback Method
tf	280.60	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.53	J/mol×K	599.91	Joback Method
cpg	722.11	J/mol×K	779.67	Joback Method
cpg	701.06	J/mol×K	743.72	Joback Method
cpg	678.52	J/mol×K	707.77	Joback Method
cpg	654.45	J/mol×K	671.81	Joback Method
cpg	628.80	J/mol×K	635.86	Joback Method
cpg	741.74	J/mol×K	815.62	Joback Method
dvisc	0.0002010	Pa×s	599.91	Joback Method

dvisc	0.0002700	Pa×s	546.69	Joback Method
dvisc	0.0003864	Pa×s	493.47	Joback Method
dvisc	0.0006031	Pa×s	440.25	Joback Method
dvisc	0.0010641	Pa×s	387.04	Joback Method
dvisc	0.0022500	Pa×s	333.82	Joback Method
dvisc	0.0063202	Pa×s	280.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54889995&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume