2-Methylbicyclohexyl

Inchi: InChI=1S/C13H24/c1-11-7-5-6-10-13(11)12-8-3-2-4-9-12/h11-13H,2-10H2,1H3
InchiKey: SRCQYSQCKOUHTG-UHFFFAOYSA-N
Formula: C13H24
SMILES: CC1CCCCC1C1CCCCC1
Mol. weight [g/mol]: 180.33
CAS: 66324-47-8

Physical Properties

Property code	Value	Unit	Source
gf	99.77	kJ/mol	Joback Method
hf	-223.35	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.393		Crippen Method
mcvol	172.310	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	523.02 ± 0.30	K	NIST Webbook
tb	528.15 ± 0.40	K	NIST Webbook
tc	758.98	K	Joback Method
tf	262.88 ± 0.30	K	NIST Webbook
tf	246.72 ± 0.20	K	NIST Webbook
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.80	J/mol×K	531.27	Joback Method
cpg	574.99	J/mol×K	758.98	Joback Method
cpg	555.70	J/mol×K	721.03	Joback Method
cpg	534.97	J/mol×K	683.08	Joback Method
cpg	512.76	J/mol×K	645.12	Joback Method
cpg	489.03	J/mol×K	607.17	Joback Method
cpg	463.72	J/mol×K	569.22	Joback Method

cpl	331.40	J/mol×K	313.00	NIST Webbook
dvisc	0.0002573	Pa×s	531.27	Joback Method
dvisc	0.0003416	Pa×s	483.86	Joback Method
dvisc	0.0004821	Pa×s	436.44	Joback Method
dvisc	0.0007403	Pa×s	389.03	Joback Method
dvisc	0.0012802	Pa×s	341.62	Joback Method
dvisc	0.0026414	Pa×s	294.20	Joback Method
dvisc	0.0071989	Pa×s	246.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66324478&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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