

Cycloheptene, 1-butyl

Inchi:	InChI=1S/C11H20/c1-2-3-8-11-9-6-4-5-7-10-11/h9H,2-8,10H2,1H3
InchiKey:	RNQIHPNBLWDWSR-UHFFFAOYSA-N
Formula:	C11H20
SMILES:	CCCCC1=CCCCC1
Mol. weight [g/mol]:	152.28

Physical Properties

Property code	Value	Unit	Source
gf	82.13	kJ/mol	Joback Method
hf	-155.56	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	41.94	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.067		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1151.00		NIST Webbook
tb	483.71	K	Joback Method
tc	689.29	K	Joback Method
tf	235.11	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.26	J/mol×K	483.71	Joback Method
cpg	351.68	J/mol×K	517.97	Joback Method
cpg	370.13	J/mol×K	552.24	Joback Method
cpg	387.61	J/mol×K	586.50	Joback Method
cpg	404.17	J/mol×K	620.76	Joback Method
cpg	419.81	J/mol×K	655.03	Joback Method
cpg	434.58	J/mol×K	689.29	Joback Method
dvisc	0.0092589	Pa×s	235.11	Joback Method
dvisc	0.0029695	Pa×s	276.54	Joback Method

dvisc	0.0012809	Pa×s	317.98	Joback Method
dvisc	0.0006707	Pa×s	359.41	Joback Method
dvisc	0.0004015	Pa×s	400.84	Joback Method
dvisc	0.0002646	Pa×s	442.28	Joback Method
dvisc	0.0001873	Pa×s	483.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R133121&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
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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