5-Butylindan

Inchi: InChI=1S/C13H18/c1-2-3-5-11-8-9-12-6-4-7-13(12)10-11/h8-10H,2-7H2,1H3
InchiKey: UJGOUXAEHNPLGZ-UHFFFAOYSA-N
Formula: C13H18
SMILES: CCCCc1ccc2c(c1)CCC2
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
gf	220.19	kJ/mol	Joback Method
hf	-4.92	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	48.35	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.518		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1430.24		NIST Webbook
rinpol	1415.33		NIST Webbook
rinpol	1443.20		NIST Webbook
rinpol	1438.14		NIST Webbook
rinpol	1410.65		NIST Webbook
rinpol	1403.33		NIST Webbook
tb	544.89	K	Joback Method
tc	758.81	K	Joback Method
tf	309.91	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.16	J/mol×K	544.89	Joback Method
cpg	396.60	J/mol×K	580.54	Joback Method
cpg	412.96	J/mol×K	616.20	Joback Method
cpg	428.30	J/mol×K	651.85	Joback Method

cpg	442.69	J/mol×K	687.50	Joback Method
cpg	456.20	J/mol×K	723.16	Joback Method
cpg	468.90	J/mol×K	758.81	Joback Method
dvisc	0.0019150	Pa×s	309.91	Joback Method
dvisc	0.0012415	Pa×s	349.07	Joback Method
dvisc	0.0008784	Pa×s	388.24	Joback Method
dvisc	0.0006622	Pa×s	427.40	Joback Method
dvisc	0.0005234	Pa×s	466.56	Joback Method
dvisc	0.0004291	Pa×s	505.73	Joback Method
dvisc	0.0003619	Pa×s	544.89	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R250632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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