5-Propylindan

Inchi: InChI=1S/C12H16/c1-2-4-10-7-8-11-5-3-6-12(11)9-10/h7-9H,2-6H2,1H3
InchiKey: SHDSHIPDVFBPHC-UHFFFAOYSA-N
Formula: C12H16
SMILES: CCCc1ccc2c(c1)CCC2
Mol. weight [g/mol]: 160.26

Physical Properties

Property code	Value	Unit	Source
gf	211.77	kJ/mol	Joback Method
hf	15.72	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.128		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1305.58		NIST Webbook
rinpol	1310.08		NIST Webbook
rinpol	1324.30		NIST Webbook
rinpol	1331.98		NIST Webbook
rinpol	1336.96		NIST Webbook
rinpol	1298.54		NIST Webbook
tb	522.01	K	Joback Method
tc	739.55	K	Joback Method
tf	298.64	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.81	J/mol×K	522.01	Joback Method
cpg	348.59	J/mol×K	558.27	Joback Method
cpg	364.30	J/mol×K	594.52	Joback Method
cpg	379.00	J/mol×K	630.78	Joback Method

cpg	392.76	J/mol×K	667.03	Joback Method
cpg	405.65	J/mol×K	703.29	Joback Method
cpg	417.73	J/mol×K	739.55	Joback Method
dvisc	0.0018136	Pa×s	298.64	Joback Method
dvisc	0.0012043	Pa×s	335.87	Joback Method
dvisc	0.0008678	Pa×s	373.10	Joback Method
dvisc	0.0006636	Pa×s	410.32	Joback Method
dvisc	0.0005306	Pa×s	447.55	Joback Method
dvisc	0.0004391	Pa×s	484.78	Joback Method
dvisc	0.0003733	Pa×s	522.01	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250652&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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