1,3-Cyclopentadiene, 2-heptyl

Inchi: InChI=1S/C12H20/c1-2-3-4-5-6-9-12-10-7-8-11-12/h7,10-11H,2-6,8-9H2,1H3
InchiKey: UWYAUNBMYZAOBX-UHFFFAOYSA-N
Formula: C12H20
SMILES: CCCCCCCC1=CCC=C1
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	144.71	kJ/mol	Joback Method
hf	-106.10	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	44.12	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.233		Crippen Method
mcvol	160.480	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
ripol	1399.40		NIST Webbook
ripol	1399.40		NIST Webbook
tb	497.21	K	Joback Method
tc	687.60	K	Joback Method
tf	254.18	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.16	J/mol×K	497.21	Joback Method
cpg	379.20	J/mol×K	528.94	Joback Method
cpg	395.37	J/mol×K	560.67	Joback Method
cpg	410.71	J/mol×K	592.41	Joback Method
cpg	425.25	J/mol×K	624.14	Joback Method
cpg	439.04	J/mol×K	655.87	Joback Method

cpg	452.10	J/mol×K	687.60	Joback Method
dvisc	0.0034483	Pa×s	254.18	Joback Method
dvisc	0.0016562	Pa×s	294.69	Joback Method
dvisc	0.0009497	Pa×s	335.19	Joback Method
dvisc	0.0006140	Pa×s	375.70	Joback Method
dvisc	0.0004321	Pa×s	416.20	Joback Method
dvisc	0.0003236	Pa×s	456.71	Joback Method
dvisc	0.0002541	Pa×s	497.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R40831&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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