

4-isopropyl-1-methylcyclohepta-1,3,5-triene

Inchi:	InChI=1S/C11H16/c1-9(2)11-6-4-5-10(3)7-8-11/h4,6-9H,5H2,1-3H3
InchiKey:	XSAARUMVRDUCPJ-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CC1=CC=C(C(C)C)C=CC1
Mol. weight [g/mol]:	148.24

Physical Properties

Property code	Value	Unit	Source
gf	129.98	kJ/mol	Joback Method
hf	-56.75	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.475		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1082.50		NIST Webbook
rinpol	1082.50		NIST Webbook
tb	486.57	K	Joback Method
tc	702.51	K	Joback Method
tf	234.15	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.71	J/molxK	486.57	Joback Method
cpg	317.82	J/molxK	522.56	Joback Method
cpg	334.01	J/molxK	558.55	Joback Method
cpg	349.31	J/molxK	594.54	Joback Method
cpg	363.74	J/molxK	630.53	Joback Method
cpg	377.32	J/molxK	666.52	Joback Method
cpg	390.09	J/molxK	702.51	Joback Method
dvisc	0.0054660	Paxs	234.15	Joback Method

dvisc	0.0019564	Paxs	276.22	Joback Method
dvisc	0.0009188	Paxs	318.29	Joback Method
dvisc	0.0005147	Paxs	360.36	Joback Method
dvisc	0.0003255	Paxs	402.43	Joback Method
dvisc	0.0002245	Paxs	444.50	Joback Method
dvisc	0.0001651	Paxs	486.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492158&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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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