(Z)-4,8-dimethylnona-1,3,7-triene

Inchi: InChI=1S/C11H18/c1-5-7-11(4)9-8-10(3)6-2/h5-7H,1,8-9H2,2-4H3/b10-6+,11-7-
InchiKey: GDFQYTBTUZEBAW-QZTBCQRESA-N
Formula: C11H18
SMILES: C=CC=C(C)CCC(C)=CC
Mol. weight [g/mol]: 150.26

Physical Properties

Property code	Value	Unit	Source
gf	272.92	kJ/mol	Joback Method
hf	69.92	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.865		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1092.00		NIST Webbook
tb	455.84	K	Joback Method
tc	643.33	K	Joback Method
tf	173.89	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.66	J/mol×K	455.84	Joback Method
cpg	327.28	J/mol×K	487.09	Joback Method
cpg	342.08	J/mol×K	518.34	Joback Method
cpg	356.08	J/mol×K	549.58	Joback Method
cpg	369.34	J/mol×K	580.83	Joback Method

cpg	381.90	J/mol×K	612.08	Joback Method
cpg	393.80	J/mol×K	643.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285435&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
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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