Isomyocorene

Other names:	2,6-Dimethyl 1,3,7-octatriene (alpha menthrene)
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5-7,10H,1-2,8H2,3-4H3/b7-6+
InchiKey:	JWMIAIJDECOUIA-VOTSOKGWSA-N
Formula:	C10H16
SMILES:	C=CC(C)CC=CC(=C)C
Mol. weight [g/mol]:	136.23
CAS:	6876-07-9

Physical Properties

Property code	Value	Unit	Source
gf	278.23	kJ/mol	Joback Method
hf	103.28	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	36.16	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.331		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
tb	425.16	K	Joback Method
tc	609.91	K	Joback Method
tf	164.90	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.01	J/mol×K	425.16	Joback Method
cpg	282.59	J/mol×K	455.95	Joback Method
cpg	296.43	J/mol×K	486.74	Joback Method
cpg	309.56	J/mol×K	517.53	Joback Method
cpg	322.00	J/mol×K	548.32	Joback Method
cpg	333.80	J/mol×K	579.12	Joback Method
cpg	344.99	J/mol×K	609.91	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=C6876079&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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