3-Methyl-4-brendene

Inchi: InChI=1S/C10H14/c1-10-3-2-8-4-7(6-10)5-9(8)10/h2-3,7-9H,4-6H2,1H3
InchiKey: YXLBQJSAWXSFAF-UHFFFAOYSA-N
Formula: C10H14
SMILES: CC12C=CC3CC(CC31)C2
Mol. weight [g/mol]: 134.22

Physical Properties

Property code	Value	Unit	Source
gf	232.33	kJ/mol	Joback Method
hf	21.35	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	36.42	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.609		Crippen Method
mcvol	114.880	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	443.15	K	Joback Method
tc	659.95	K	Joback Method
tf	276.70	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.94	J/mol×K	443.15	Joback Method
cpg	278.18	J/mol×K	479.28	Joback Method
cpg	295.66	J/mol×K	515.42	Joback Method
cpg	311.60	J/mol×K	551.55	Joback Method
cpg	326.17	J/mol×K	587.68	Joback Method
cpg	339.58	J/mol×K	623.81	Joback Method
cpg	352.02	J/mol×K	659.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R440078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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