9-Methylretene

Inchi: InChI=1S/C19H20/c1-12(2)15-8-9-17-16-7-5-6-13(3)18(16)10-14(4)19(17)11-15/h5-12H,
InchiKey: XEDSPKKJZIHGDE-UHFFFAOYSA-N
Formula: C19H20
SMILES: Cc1cc2c(C)cccc2c2ccc(C(C)C)cc12
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	393.85	kJ/mol	Joback Method
hf	132.02	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.733		Crippen Method
mcvol	215.890	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	367.36		NIST Webbook
rinpol	370.31		NIST Webbook
rinpol	370.31		NIST Webbook
tb	718.24	K	Joback Method
tc	953.58	K	Joback Method
tf	430.79	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.55	J/mol×K	718.24	Joback Method
cpg	661.00	J/mol×K	914.36	Joback Method
cpg	647.70	J/mol×K	875.14	Joback Method
cpg	633.61	J/mol×K	835.91	Joback Method
cpg	618.63	J/mol×K	796.69	Joback Method
cpg	602.65	J/mol×K	757.46	Joback Method
cpg	673.62	J/mol×K	953.58	Joback Method

dvisc	0.0003362	Pa×s	718.24	Joback Method
dvisc	0.0003853	Pa×s	670.33	Joback Method
dvisc	0.0004510	Pa×s	622.42	Joback Method
dvisc	0.0005419	Pa×s	574.52	Joback Method
dvisc	0.0006732	Pa×s	526.61	Joback Method
dvisc	0.0008735	Pa×s	478.70	Joback Method
dvisc	0.0012010	Pa×s	430.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R278576&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume