Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)-

Other names: Cyclotetradecane, 4-isopropyl-1,7,11-trimethyl-
Cembrane
Cembrene, octahydro-

Inchi: InChI=1S/C20H40/c1-16(2)20-14-12-18(4)10-6-8-17(3)9-7-11-19(5)13-15-20/h16-20H,6-

InchiKey: LHORCXXUZJAMPU-UHFFFAOYSA-N

Formula: C20H40

SMILES: CC1CCCC(C)CCC(C(C)C)CCC(C)CCC1

Mol. weight [g/mol]: 280.53

CAS: 1786-12-5

Physical Properties

Property code	Value	Unit	Source
gf	19.60	kJ/mol	Joback Method
hf	-517.39	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	60.60	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	7.082		Crippen Method
mcvol	281.800	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
tb	696.26	K	Joback Method
tc	921.11	K	Joback Method
tf	266.66	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.31	J/mol×K	696.26	Joback Method
cpg	906.80	J/mol×K	733.73	Joback Method
cpg	937.03	J/mol×K	771.21	Joback Method
cpg	964.97	J/mol×K	808.68	Joback Method
cpg	990.60	J/mol×K	846.16	Joback Method
cpg	1013.89	J/mol×K	883.63	Joback Method

cpg	1034.81	J/mol×K	921.11	Joback Method
dvisc	0.0301854	Pa×s	266.66	Joback Method
dvisc	0.0021647	Pa×s	338.26	Joback Method
dvisc	0.0003898	Pa×s	409.86	Joback Method
dvisc	0.0001169	Pa×s	481.46	Joback Method
dvisc	0.0000479	Pa×s	553.06	Joback Method
dvisc	0.0000241	Pa×s	624.66	Joback Method
dvisc	0.0000139	Pa×s	696.26	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=C1786125&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume