3,7,11,15-Tetramethyl-2-hexadecene

Inchi: InChI=1S/C20H40/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,17,19-20H,8
InchiKey: XZJQZWIDAHFTHV-UHFFFAOYSA-N
Formula: C20H40
SMILES: CC=C(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 280.53

Physical Properties

Property code	Value	Unit	Source
gf	181.87	kJ/mol	Joback Method
hf	-364.54	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	7.392		Crippen Method
mcvol	288.360	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
rinpol	1838.00		NIST Webbook
rinpol	1854.00		NIST Webbook
rinpol	1838.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	659.72	K	Joback Method
tc	831.83	K	Joback Method
tf	251.12	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.64	J/mol×K	659.72	Joback Method
cpg	842.22	J/mol×K	688.41	Joback Method
cpg	862.81	J/mol×K	717.09	Joback Method
cpg	882.47	J/mol×K	745.78	Joback Method

cpg	901.23	J/mol×K	774.46	Joback Method
cpg	919.14	J/mol×K	803.15	Joback Method
cpg	936.22	J/mol×K	831.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285871&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume