3,7,11,15-Tetramethyl-2-hexadecen-1-ol

Other names: 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl
Inchi: InChI=1S/C20H40O/c1-17(2)9-6-10-18(3)11-7-12-19(4)13-8-14-20(5)15-16-21/h15,17-19
InchiKey: BOTWFXYSPFMFNR-UHFFFAOYSA-N
Formula: C20H40O
SMILES: CC(=CCO)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 296.53
CAS: 102608-53-7

Physical Properties

Property code	Value	Unit	Source
gf	45.05	kJ/mol	Joback Method
hf	-516.77	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.364		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	2119.33		NIST Webbook
rinpol	2119.33		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	751.90	K	Joback Method
tc	926.94	K	Joback Method
tf	311.94	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.37	J/mol×K	751.90	Joback Method
cpg	923.39	J/mol×K	781.07	Joback Method
cpg	941.52	J/mol×K	810.25	Joback Method
cpg	958.79	J/mol×K	839.42	Joback Method

cpg	975.26	J/mol×K	868.59	Joback Method
cpg	990.97	J/mol×K	897.76	Joback Method
cpg	1005.95	J/mol×K	926.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102608537&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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