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

Inchi: InChI=1S/C20H40O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h7,17-19,2
InchiKey: KEVYVLWNCKMXJX-UHFFFAOYSA-N
Formula: C20H40O
SMILES: C=CC(C)(O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 296.53
CAS: 60046-87-9

Physical Properties

Property code	Value	Unit	Source
gf	64.06	kJ/mol	Joback Method
hf	-507.52	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.362		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
tb	741.31	K	Joback Method
tc	916.20	K	Joback Method
tf	331.64	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.43	J/mol×K	887.05	Joback Method
cpg	903.98	J/mol×K	741.31	Joback Method
cpg	923.04	J/mol×K	770.46	Joback Method
cpg	941.17	J/mol×K	799.61	Joback Method
cpg	958.41	J/mol×K	828.75	Joback Method
cpg	974.81	J/mol×K	857.90	Joback Method
cpg	1005.31	J/mol×K	916.20	Joback Method
cpl	729.50	J/mol×K	293.75	NIST Webbook
dvisc	0.0000137	Pa×s	741.31	Joback Method

dvisc	0.0150671	Pa×s	331.64	Joback Method
dvisc	0.0017320	Pa×s	399.92	Joback Method
dvisc	0.0003742	Pa×s	468.20	Joback Method
dvisc	0.0001194	Pa×s	536.47	Joback Method
dvisc	0.0000493	Pa×s	604.75	Joback Method
dvisc	0.0000244	Pa×s	673.03	Joback Method
hvapt	67.00 ± 2.00	kJ/mol	453.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31485e+01
Coeff. B	-4.77767e+03
Coeff. C	-1.16172e+02
Temperature range (K), min.	487.66
Temperature range (K), max.	725.80

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=C60046879&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

cpl: Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume