3,7,11,15-Tetramethylhexadecene, isomer 3

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	1880.00		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

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=R573376&Units=SI

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