Hexadecane, 2,6,14-trimethyl

Inchi: InChI=1S/C19H40/c1-6-18(4)14-10-8-7-9-11-15-19(5)16-12-13-17(2)3/h17-19H,6-16H2,1
InchiKey: NBXARZKUSHAIJP-UHFFFAOYSA-N
Formula: C19H40
SMILES: CCC(C)CCCCCCCC(C)CCCC(C)C
Mol. weight [g/mol]: 268.52

Physical Properties

Property code	Value	Unit	Source
gf	101.78	kJ/mol	Joback Method
hf	-451.33	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	56.72	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	7.226		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	632.80	K	Joback Method
tc	798.17	K	Joback Method
tf	258.89	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.31	J/mol×K	632.80	Joback Method
cpg	803.70	J/mol×K	660.36	Joback Method
cpg	824.19	J/mol×K	687.92	Joback Method
cpg	843.79	J/mol×K	715.49	Joback Method
cpg	862.54	J/mol×K	743.05	Joback Method
cpg	880.46	J/mol×K	770.61	Joback Method

cpg	897.59	J/mol×K	798.17	Joback Method
dvisc	0.0137841	Pa×s	258.89	Joback Method
dvisc	0.0026251	Pa×s	321.21	Joback Method
dvisc	0.0008570	Pa×s	383.53	Joback Method
dvisc	0.0003826	Pa×s	445.84	Joback Method
dvisc	0.0002081	Pa×s	508.16	Joback Method
dvisc	0.0001294	Pa×s	570.48	Joback Method
dvisc	0.0000883	Pa×s	632.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R12159&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
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
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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