Hexadecane, 8-ethyl

Inchi: InChI=1S/C19H40/c1-4-7-9-11-12-14-16-18-19(6-3)17-15-13-10-8-5-2/h19H,4-18H2,1-3H
InchiKey: PFHNDLOOIBCYQP-UHFFFAOYSA-N
Formula: C19H40
SMILES: CCCCCCCCCC(CC)CCCCCCC
Mol. weight [g/mol]: 268.52

Physical Properties

Property code	Value	Unit	Source
gf	106.66	kJ/mol	Joback Method
hf	-440.77	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.514		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1727.00		NIST Webbook
tb	633.68	K	Joback Method
tc	794.96	K	Joback Method
tf	288.89	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.70	J/mol×K	633.68	Joback Method
cpg	877.35	J/mol×K	768.08	Joback Method
cpg	859.82	J/mol×K	741.20	Joback Method
cpg	841.51	J/mol×K	714.32	Joback Method
cpg	822.41	J/mol×K	687.44	Joback Method
cpg	802.48	J/mol×K	660.56	Joback Method

cpg	894.13	J/mol×K	794.96	Joback Method
dvisc	0.0001019	Pa×s	633.68	Joback Method
dvisc	0.0001427	Pa×s	576.22	Joback Method
dvisc	0.0002152	Pa×s	518.75	Joback Method
dvisc	0.0003595	Pa×s	461.29	Joback Method
dvisc	0.0006952	Pa×s	403.82	Joback Method
dvisc	0.0016729	Pa×s	346.36	Joback Method
dvisc	0.0057089	Pa×s	288.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R8787&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

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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