Heptadecane, 7-methyl-

Other names: 7-Methylheptadecane
Inchi: InChI=1S/C18H38/c1-4-6-8-10-11-12-13-15-17-18(3)16-14-9-7-5-2/h18H,4-17H2,1-3H3
InchiKey: AZGIFKCGYRMPKP-UHFFFAOYSA-N
Formula: C18H38
SMILES: CCCCCCCCCCC(C)CCCCCC
Mol. weight [g/mol]: 254.49
CAS: 20959-33-5

Physical Properties

Property code	Value	Unit	Source
gf	98.24	kJ/mol	Joback Method
hf	-420.13	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	7.124		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1746.90		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	610.80	K	Joback Method
tc	771.74	K	Joback Method
tf	277.62	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.79	J/mol×K	610.80	Joback Method

cpg	744.17	J/mol×K	637.62	Joback Method
cpg	763.72	J/mol×K	664.45	Joback Method
cpg	782.48	J/mol×K	691.27	Joback Method
cpg	800.46	J/mol×K	718.09	Joback Method
cpg	817.70	J/mol×K	744.91	Joback Method
cpg	834.20	J/mol×K	771.74	Joback Method
dvisc	0.0063506	Pa×s	277.62	Joback Method
dvisc	0.0018624	Pa×s	333.15	Joback Method
dvisc	0.0007754	Pa×s	388.68	Joback Method
dvisc	0.0004019	Pa×s	444.21	Joback Method
dvisc	0.0002411	Pa×s	499.74	Joback Method
dvisc	0.0001602	Pa×s	555.27	Joback Method
dvisc	0.0001146	Pa×s	610.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20959335&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