6-methylheptadecane

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

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	1749.70		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1749.00		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

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=R47497&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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