

6-methyltetradecane

Other names:	6-Methyltetradecane
Inchi:	InChI=1S/C15H32/c1-4-6-8-9-10-12-14-15(3)13-11-7-5-2/h15H,4-14H2,1-3H3
InchiKey:	ONQXEQPEKDADGM-UHFFFAOYSA-N
Formula:	C15H32
SMILES:	CCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	212.41
CAS:	26730-16-5

Physical Properties

Property code	Value	Unit	Source
af	0.6403		Cheméo Relay (1.0)
gf	72.98	kJ/mol	Joback Method
hf	-360.70	kJ/mol	Cheméo Relay (1.0)
hfus	31.08	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-7.20		Cheméo Relay (1.0)
logp	5.953		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
tb	526.45	K	Cheméo Relay (1.0)
tc	689.77	K	Cheméo Relay (1.0)
tf	237.80 ± 2.00	K	NIST Webbook
vc	0.864	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.22	J/mol×K	542.16	Joback Method
cpg	577.24	J/mol×K	569.12	Joback Method
cpg	595.52	J/mol×K	596.08	Joback Method
cpg	613.07	J/mol×K	623.04	Joback Method
cpg	629.92	J/mol×K	650.00	Joback Method
cpg	646.08	J/mol×K	676.97	Joback Method

cpg	661.59	J/mol×K	703.93	Joback Method
dvisc	0.0083877	Pa×s	243.81	Joback Method
dvisc	0.0024681	Pa×s	293.53	Joback Method
dvisc	0.0010352	Pa×s	343.26	Joback Method
dvisc	0.0005409	Pa×s	392.99	Joback Method
dvisc	0.0003270	Pa×s	442.71	Joback Method
dvisc	0.0002189	Pa×s	492.43	Joback Method
dvisc	0.0001577	Pa×s	542.16	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C26730165&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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