Hexacontane

Inchi: InChI=1S/C60H122/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45
InchiKey: OCWUCHKZAHTZAB-UHFFFAOYSA-N
Formula: C60H122
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 843.61
CAS: 7667-80-3

Physical Properties

Property code	Value	Unit	Source
gf	454.32	kJ/mol	Joback Method
hf	-1281.73	kJ/mol	Joback Method
hfus	151.16	kJ/mol	Joback Method
hvap	299.90 ± 2.00	kJ/mol	NIST Webbook
log10ws	-24.94		Crippen Method
logp	23.652		Crippen Method
mcvol	856.260	ml/mol	McGowan Method
pc	205.37	kPa	Joback Method
tb	1572.20	K	Joback Method
tc	974.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	375.00 ± 4.00	K	NIST Webbook
tf	375.00 ± 4.00	K	NIST Webbook
tf	372.10 ± 2.00	K	NIST Webbook
tf	375.00 ± 2.00	K	NIST Webbook
vc	3.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	10341.68	J/mol×K	3498.85	Joback Method
cpg	5663.66	J/mol×K	2728.19	Joback Method
cpg	4564.18	J/mol×K	2342.86	Joback Method

cpg	3969.36	J/mol×K	1957.53	Joback Method
cpg	3637.97	J/mol×K	1572.20	Joback Method
cpg	7509.08	J/mol×K	3113.52	Joback Method
cpg	14402.72	J/mol×K	3884.17	Joback Method
dvisc	0.0000086	Pa×s	765.96	Joback Method
dvisc	0.0000002	Pa×s	1572.20	Joback Method
dvisc	0.0000002	Pa×s	1437.83	Joback Method
dvisc	0.0000003	Pa×s	1303.45	Joback Method
dvisc	0.0000006	Pa×s	1169.08	Joback Method
dvisc	0.0000011	Pa×s	1034.71	Joback Method
dvisc	0.0000027	Pa×s	900.33	Joback Method
hfust	186.80	kJ/mol	373.20	NIST Webbook
hvapt	163.00	kJ/mol	765.50	NIST Webbook
hvapt	299.90	kJ/mol	298.15	Hypothetical Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even n-Alkanes from C40 to C76 at T = 298.15 K by Correlation-Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique:	https://www.doi.org/10.1016/j.fluid.2014.07.017
Hypothetical Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even n-Alkanes from C40 to C76 at T = 298.15 K by Correlation-Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?:	https://www.doi.org/10.1021/je7005852
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=C7667803&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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