octapentacontane

Inchi:	InChI=1S/C58H118/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45
InchiKey:	HDKSWQPFGWHOIA-UHFFFAOYSA-N
Formula:	C58H118
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	815.56
CAS:	7667-78-9

Physical Properties

Property code	Value	Unit	Source
gf	437.48	kJ/mol	Joback Method
hf	-1240.45	kJ/mol	Joback Method
hfus	145.98	kJ/mol	Joback Method
hvap	288.50 ± 1.80	kJ/mol	NIST Webbook
log10ws	-24.10		Crippen Method
logp	22.872		Crippen Method
mcvol	828.080	ml/mol	McGowan Method
pc	217.16	kPa	Joback Method
tb	1526.44	K	Joback Method
tc	3378.06	K	Joback Method
tf	370.00 ± 2.00	K	NIST Webbook
tf	373.00 ± 5.00	K	NIST Webbook
vc	3.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	7008.01	J/mol×K	3069.45	Joback Method
cpg	9017.01	J/mol×K	3378.06	Joback Method
cpg	3485.44	J/mol×K	1526.44	Joback Method
cpg	3719.42	J/mol×K	1835.04	Joback Method
cpg	4068.92	J/mol×K	2143.65	Joback Method
cpg	4653.70	J/mol×K	2452.25	Joback Method
cpg	5593.49	J/mol×K	2760.85	Joback Method
dvisc	0.0000002	Pa×s	1526.44	Joback Method

dvisc	0.0000003	Pa×s	1395.94	Joback Method
dvisc	0.0000122	Pa×s	743.42	Joback Method
dvisc	0.0000038	Pa×s	873.92	Joback Method
dvisc	0.0000016	Pa×s	1004.43	Joback Method
dvisc	0.0000008	Pa×s	1134.93	Joback Method
dvisc	0.0000005	Pa×s	1265.43	Joback Method
hvapt	160.30	kJ/mol	759.00	NIST Webbook
hvapt	288.50	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7667789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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
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