

Hexatetracontane

Inchi: InChI=1S/C46H94/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45-47
InchiKey: PVQAQPUODMPGGG-UHFFFAOYSA-N
Formula: C46H94
SMILES: CC
Mol. weight [g/mol]: 647.24
CAS: 7098-24-0

Physical Properties

Property code	Value	Unit	Source
gf	336.44	kJ/mol	Joback Method
hf	-992.77	kJ/mol	Joback Method
hfus	114.90	kJ/mol	Joback Method
hvap	233.30	kJ/mol	NIST Webbook
log10ws	-19.08		Crippen Method
logp	18.191		Crippen Method
mcvol	659.000	ml/mol	McGowan Method
pc	315.04	kPa	Joback Method
tb	1251.88	K	Joback Method
tc	1856.15	K	Joback Method
tf	361.00 ± 4.00	K	NIST Webbook
tf	361.00 ± 2.00	K	NIST Webbook
vc	2.611	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2901.69	J/molxK	1755.44	Joback Method
cpg	2841.31	J/molxK	1654.72	Joback Method
cpg	2784.66	J/molxK	1554.01	Joback Method
cpg	2728.43	J/molxK	1453.30	Joback Method
cpg	2669.35	J/molxK	1352.59	Joback Method
cpg	2604.12	J/molxK	1251.88	Joback Method
cpg	2969.06	J/molxK	1856.15	Joback Method
dvisc	0.0000923	Paxs	608.18	Joback Method

dvisc	0.0000018	Paxs	1251.88	Joback Method
dvisc	0.0000026	Paxs	1144.60	Joback Method
dvisc	0.0000039	Paxs	1037.31	Joback Method
dvisc	0.0000066	Paxs	930.03	Joback Method
dvisc	0.0000126	Paxs	822.75	Joback Method
dvisc	0.0000294	Paxs	715.46	Joback Method
hfust	151.40	kJ/mol	360.70	NIST Webbook
hvapt	142.80	kJ/mol	709.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7098240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
mccvol:	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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