

Tetratriacontane, 11,15,19-trimethyl

Inchi: InChI=1S/C47H96/c1-6-8-10-12-14-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-32-34-35-36-37-38-39-40-41-42-43-44-45-46-47
InchiKey: MKNMNJAAFBOQCD-UHFFFAOYSA-N
Formula: C47H96
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]: 661.27

Physical Properties

Property code	Value	Unit	Source
gf	337.54	kJ/mol	Joback Method
hf	-1029.25	kJ/mol	Joback Method
hfus	106.92	kJ/mol	Joback Method
hvap	119.05	kJ/mol	Joback Method
log10ws	-18.77		Crippen Method
logp	18.148		Crippen Method
mcvol	673.090	ml/mol	McGowan Method
pc	307.14	kPa	Joback Method
rinpol	3482.00		NIST Webbook
tb	1273.44	K	Joback Method
tc	1881.82	K	Joback Method
tf	574.45	K	Joback Method
vc	2.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2674.10	J/mol×K	1273.44	Joback Method
cpg	2737.94	J/mol×K	1374.84	Joback Method
cpg	2795.86	J/mol×K	1476.23	Joback Method
cpg	2851.27	J/mol×K	1577.63	Joback Method
cpg	2907.59	J/mol×K	1679.03	Joback Method
cpg	2968.25	J/mol×K	1780.43	Joback Method
cpg	3036.66	J/mol×K	1881.82	Joback Method
dvisc	0.0001161	Pa×s	574.45	Joback Method
dvisc	0.0000280	Pa×s	690.95	Joback Method

dvisc	0.0000102	Pa×s	807.45	Joback Method
dvisc	0.0000048	Pa×s	923.94	Joback Method
dvisc	0.0000026	Pa×s	1040.44	Joback Method
dvisc	0.0000017	Pa×s	1156.94	Joback Method
dvisc	0.0000011	Pa×s	1273.44	Joback Method

Sources

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=R584608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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