

6,10,12,16-Tetramethylhexatriacontane

Inchi: InChI=1S/C40H82/c1-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-27-31-38(4)33
InchiKey: YHNFOHKDNXSTMM-UHFFFAOYSA-N
Formula: C40H82
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CC(C)CCCC(C)CCCC
Mol. weight [g/mol]: 563.08

Physical Properties

Property code	Value	Unit	Source
gf	276.16	kJ/mol	Joback Method
hf	-890.05	kJ/mol	Joback Method
hfus	85.26	kJ/mol	Joback Method
hvap	103.08	kJ/mol	Joback Method
log10ws	-15.60		Crippen Method
logp	15.274		Crippen Method
mcvol	574.460	ml/mol	McGowan Method
pc	395.87	kPa	Joback Method
rinpol	3723.00		NIST Webbook
rinpol	3723.00		NIST Webbook
rinpol	3723.00		NIST Webbook
tb	1112.84	K	Joback Method
tc	1460.95	K	Joback Method
tf	480.56	K	Joback Method
vc	2.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2175.86	J/molxK	1112.84	Joback Method
cpg	2216.12	J/molxK	1170.86	Joback Method
cpg	2252.75	J/molxK	1228.88	Joback Method
cpg	2286.29	J/molxK	1286.90	Joback Method
cpg	2317.29	J/molxK	1344.92	Joback Method
cpg	2346.28	J/molxK	1402.93	Joback Method
cpg	2373.80	J/molxK	1460.95	Joback Method

dvisc	0.0004973	Paxs	480.56	Joback Method
dvisc	0.0001022	Paxs	585.94	Joback Method
dvisc	0.0000340	Paxs	691.32	Joback Method
dvisc	0.0000152	Paxs	796.70	Joback Method
dvisc	0.0000082	Paxs	902.08	Joback Method
dvisc	0.0000050	Paxs	1007.46	Joback Method
dvisc	0.0000034	Paxs	1112.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R505690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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