5,21-dimethylpentatriacontane

Inchi: InChI=1S/C37H76/c1-5-7-9-10-11-12-13-17-20-24-27-30-34-37(4)35-31-28-25-22-19-16-
InchiKey: IRULTYNWOAKUPO-UHFFFAOYSA-N
Formula: C37H76
SMILES: CCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 521.00

Physical Properties

Property code	Value	Unit	Source
gf	255.78	kJ/mol	Joback Method
hf	-817.57	kJ/mol	Joback Method
hfus	84.54	kJ/mol	Joback Method
hvap	97.18	kJ/mol	Joback Method
log10ws	-14.83		Crippen Method
logp	14.391		Crippen Method
mcvol	532.190	ml/mol	McGowan Method
pc	442.47	kPa	Joback Method
rinpol	3583.00		NIST Webbook
rinpol	3583.00		NIST Webbook
rinpol	3583.00		NIST Webbook
tb	1045.08	K	Joback Method
tc	1340.34	K	Joback Method
tf	476.75	K	Joback Method
vc	2.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1965.02	J/mol×K	1045.08	Joback Method
cpg	2119.51	J/mol×K	1291.13	Joback Method
cpg	2093.10	J/mol×K	1241.92	Joback Method
cpg	2064.75	J/mol×K	1192.71	Joback Method
cpg	2034.16	J/mol×K	1143.50	Joback Method
cpg	2001.02	J/mol×K	1094.29	Joback Method
cpg	2144.28	J/mol×K	1340.34	Joback Method

dvisc	0.0000067	Pa×s	1045.08	Joback Method
dvisc	0.0000097	Pa×s	950.36	Joback Method
dvisc	0.0000152	Pa×s	855.64	Joback Method
dvisc	0.0000267	Pa×s	760.91	Joback Method
dvisc	0.0000550	Pa×s	666.19	Joback Method
dvisc	0.0001441	Pa×s	571.47	Joback Method
dvisc	0.0005532	Pa×s	476.75	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=R272563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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