Tritriacontane, 13,17-dimethyl

Other names: Tritriacontane, 13,17-dimethyl
Inchi: InChI=1S/C35H72/c1-5-7-9-11-13-15-17-18-19-20-22-24-26-28-31-35(4)33-29-32-34(3)3
InchiKey: NAIVJVHYZWMQFH-UHFFFAOYSA-N
Formula: C35H72
SMILES: CCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 492.96

Physical Properties

Property code	Value	Unit	Source
af	1.2997		Cheméo Relay (1.0)
gf	238.94	kJ/mol	Joback Method
hf	-797.58	kJ/mol	Cheméo Relay (1.0)
hfus	79.36	kJ/mol	Joback Method
hvap	164.03	kJ/mol	Cheméo Relay (1.0)
ie	10.08	eV	Cheméo Relay (1.0)
log10ws	-12.58		Cheméo Relay (1.0)
logp	13.611		Crippen Method
mcvol	504.010	ml/mol	McGowan Method
pc	480.50	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3352.00		NIST Webbook
rinpol	3359.00		NIST Webbook
tb	671.82	K	Cheméo Relay (1.0)
tc	841.30	K	Cheméo Relay (1.0)
tf	291.75	K	Cheméo Relay (1.0)
vc	1.966	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1825.56	J/mol×K	999.32	Joback Method
cpg	1858.31	J/mol×K	1042.84	Joback Method
cpg	1888.72	J/mol×K	1086.36	Joback Method
cpg	1916.96	J/mol×K	1129.87	Joback Method

cpg	1943.25	J/mol×K	1173.39	Joback Method
cpg	1967.79	J/mol×K	1216.91	Joback Method
cpg	1990.77	J/mol×K	1260.43	Joback Method
dvisc	0.0007702	Pa×s	454.21	Joback Method
dvisc	0.0001994	Pa×s	545.06	Joback Method
dvisc	0.0000760	Pa×s	635.91	Joback Method
dvisc	0.0000368	Pa×s	726.76	Joback Method
dvisc	0.0000210	Pa×s	817.62	Joback Method
dvisc	0.0000134	Pa×s	908.47	Joback Method
dvisc	0.0000093	Pa×s	999.32	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R261553&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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