

11,15-DIMETHYLTRITRIACONTANE

Other names:	Tritriacontane, 11,15-dimethyl
Inchi:	InChI=1S/C35H72/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-24-26-28-31-35(4)33-29-32-
InchiKey:	IDJYSQCASWJCLM-UHFFFAOYSA-N
Formula:	C35H72
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCC
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	3352.00		NIST Webbook
rinpol	3363.00		NIST Webbook
rinpol	3344.00		NIST Webbook
rinpol	3355.00		NIST Webbook
rinpol	3363.00		NIST Webbook
rinpol	3343.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3344.00		NIST Webbook
rinpol	3355.00		NIST Webbook
rinpol	3359.00		NIST Webbook
rinpol	3345.00		NIST Webbook
rinpol	3354.00		NIST Webbook
rinpol	3355.00		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

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=C56987781&Units=SI
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

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

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