

Tritriacontane, 7,11-dimethyl

Inchi: InChI=1S/C35H72/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-28-31-35
InchiKey: LWHLOZMGRGBXOI-UHFFFAOYSA-N
Formula: C35H72
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCC
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	164.05	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	3363.00		NIST Webbook
rinpol	3370.00		NIST Webbook
rinpol	3363.00		NIST Webbook
tb	671.79	K	Cheméo Relay (1.0)
tc	841.31	K	Cheméo Relay (1.0)
tf	291.59	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=R300579&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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