11-Triacontene

Inchi: InChI=1S/C33H66/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-32-30-28-26-24-22-
InchiKey: KRPBUCCMJRLVLS-XTQSDGFTSA-N
Formula: C33H66
SMILES: CCCCCCCCCCC=CCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 462.88

Physical Properties

Property code	Value	Unit	Source
gf	307.20	kJ/mol	Joback Method
hf	-607.23	kJ/mol	Joback Method
hfus	81.43	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-13.49		Crippen Method
logp	12.895		Crippen Method
mcvol	471.530	ml/mol	McGowan Method
pc	532.38	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	958.60	K	Joback Method
tc	1194.51	K	Joback Method
tf	456.59	K	Joback Method
vc	1.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1659.81	J/mol×K	958.60	Joback Method
cpg	1793.25	J/mol×K	1155.20	Joback Method
cpg	1769.47	J/mol×K	1115.88	Joback Method
cpg	1744.39	J/mol×K	1076.56	Joback Method
cpg	1717.86	J/mol×K	1037.24	Joback Method
cpg	1689.72	J/mol×K	997.92	Joback Method
cpg	1815.89	J/mol×K	1194.51	Joback Method
dvisc	0.0000134	Pa×s	958.60	Joback Method

dvisc	0.0000189	Pa×s	874.93	Joback Method
dvisc	0.0000284	Pa×s	791.26	Joback Method
dvisc	0.0000472	Pa×s	707.59	Joback Method
dvisc	0.0000898	Pa×s	623.93	Joback Method
dvisc	0.0002085	Pa×s	540.26	Joback Method
dvisc	0.0006594	Pa×s	456.59	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=R528024&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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