

Tritriacont-9-ene

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:	BMSAQLIFYCSRH-HTXNQAPBSA-N
Formula:	C33H66
SMILES:	CCCCCCCC=CCCCCCCCCCCCCCCCCCCCCCCC
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
mvol	471.530	ml/mol	McGowan Method
pc	532.38	kPa	Joback Method
rinpol	3277.00		NIST Webbook
tb	958.60	K	Joback Method
tc	1194.51	K	Joback Method
tf	456.59	K	Joback Method
vc	1.863	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1659.81	J/molxK	958.60	Joback Method
cpg	1689.72	J/molxK	997.92	Joback Method
cpg	1717.86	J/molxK	1037.24	Joback Method
cpg	1744.39	J/molxK	1076.56	Joback Method
cpg	1769.47	J/molxK	1115.88	Joback Method
cpg	1793.25	J/molxK	1155.20	Joback Method
cpg	1815.89	J/molxK	1194.51	Joback Method
dvisc	0.0006594	Paxs	456.59	Joback Method
dvisc	0.0002085	Paxs	540.26	Joback Method

dvisc	0.0000898	Paxs	623.93	Joback Method
dvisc	0.0000472	Paxs	707.59	Joback Method
dvisc	0.0000284	Paxs	791.26	Joback Method
dvisc	0.0000189	Paxs	874.93	Joback Method
dvisc	0.0000134	Paxs	958.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R418150&Units=SI

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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