

1-Methoxy-28-methylhentriacontane

Inchi:	InChI=1S/C33H68O/c1-4-30-33(2)31-28-26-24-22-20-18-16-14-12-10-8-6-5-7-9-11-13-15
InchiKey:	HYQXPMVPGWHITEJ-UHFFFAOYSA-N
Formula:	C33H68O
SMILES:	CCCC(C)CCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	480.89

Physical Properties

Property code	Value	Unit	Source
gf	119.54	kJ/mol	Joback Method
hf	-861.95	kJ/mol	Joback Method
hfus	78.89	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-12.48		Crippen Method
logp	12.212		Crippen Method
mcvol	481.700	ml/mol	McGowan Method
pc	517.70	kPa	Joback Method
rinpol	3392.00		NIST Webbook
tb	976.42	K	Joback Method
tc	1225.28	K	Joback Method
tf	468.90	K	Joback Method
vc	1.895	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1723.20	J/molxK	976.42	Joback Method
cpg	1854.47	J/molxK	1183.80	Joback Method
cpg	1832.25	J/molxK	1142.32	Joback Method
cpg	1808.15	J/molxK	1100.85	Joback Method
cpg	1782.04	J/molxK	1059.37	Joback Method
cpg	1753.77	J/molxK	1017.90	Joback Method
cpg	1874.95	J/molxK	1225.28	Joback Method
dvisc	0.0000102	Paxs	976.42	Joback Method
dvisc	0.0000145	Paxs	891.83	Joback Method

dvisc	0.0000221	Paxs	807.25	Joback Method
dvisc	0.0000371	Paxs	722.66	Joback Method
dvisc	0.0000715	Paxs	638.07	Joback Method
dvisc	0.0001683	Paxs	553.49	Joback Method
dvisc	0.0005402	Paxs	468.90	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=R547298&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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