

Butyl triacontyl ether

Inchi:	InChI=1S/C34H70O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey:	GLUBQJZBGCPZIJ-UHFFFAOYSA-N
Formula:	C34H70O
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCC
Mol. weight [g/mol]:	494.92

Physical Properties

Property code	Value	Unit	Source
gf	130.40	kJ/mol	Joback Method
hf	-877.31	kJ/mol	Joback Method
hfus	85.00	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-13.14		Crippen Method
logp	12.746		Crippen Method
mvol	495.790	ml/mol	McGowan Method
pc	494.05	kPa	Joback Method
rinpol	3465.00		NIST Webbook
rinpol	3465.00		NIST Webbook
tb	999.74	K	Joback Method
tc	1267.39	K	Joback Method
tf	495.17	K	Joback Method
vc	1.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1791.73	J/molxK	999.74	Joback Method
cpg	1824.14	J/molxK	1044.35	Joback Method
cpg	1853.96	J/molxK	1088.96	Joback Method
cpg	1881.35	J/molxK	1133.57	Joback Method
cpg	1906.50	J/molxK	1178.17	Joback Method
cpg	1929.58	J/molxK	1222.78	Joback Method
cpg	1950.79	J/molxK	1267.39	Joback Method
dvisc	0.0003895	Paxs	495.17	Joback Method

dvisc	0.0001342	Paxs	579.26	Joback Method
dvisc	0.0000606	Paxs	663.36	Joback Method
dvisc	0.0000327	Paxs	747.45	Joback Method
dvisc	0.0000200	Paxs	831.55	Joback Method
dvisc	0.0000134	Paxs	915.64	Joback Method
dvisc	0.0000096	Paxs	999.74	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=U406412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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