

Butyl tetratriacontyl ether

Inchi: InChI=1S/C38H78O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: LQBRCUVAKCXFPQ-UHFFFAOYSA-N
Formula: C38H78O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCC
Mol. weight [g/mol]: 551.03

Physical Properties

Property code	Value	Unit	Source
gf	164.08	kJ/mol	Joback Method
hf	-959.87	kJ/mol	Joback Method
hfus	95.36	kJ/mol	Joback Method
hvap	102.59	kJ/mol	Joback Method
log10ws	-14.82		Crippen Method
logp	14.306		Crippen Method
mcvol	552.150	ml/mol	McGowan Method
pc	419.40	kPa	Joback Method
rinpol	3892.00		NIST Webbook
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tb	1091.26	K	Joback Method
tc	1440.03	K	Joback Method
tf	540.25	K	Joback Method
vc	2.182	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2069.20	J/mol×K	1091.26	Joback Method
cpg	2229.43	J/mol×K	1381.90	Joback Method
cpg	2203.68	J/mol×K	1323.77	Joback Method
cpg	2175.24	J/mol×K	1265.64	Joback Method
cpg	2143.65	J/mol×K	1207.52	Joback Method
cpg	2108.45	J/mol×K	1149.39	Joback Method
cpg	2252.94	J/mol×K	1440.03	Joback Method
dvisc	0.0000050	Pa×s	1091.26	Joback Method

dvisc	0.0000070	Pa×s	999.42	Joback Method
dvisc	0.0000106	Pa×s	907.59	Joback Method
dvisc	0.0000174	Pa×s	815.75	Joback Method
dvisc	0.0000324	Pa×s	723.92	Joback Method
dvisc	0.0000724	Pa×s	632.09	Joback Method
dvisc	0.0002129	Pa×s	540.25	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=U406414&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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