

Heptyl triacontyl ether

Inchi: InChI=1S/C37H76O/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37
InchiKey: PMRCTAFTBKHUQL-UHFFFAOYSA-N
Formula: C37H76O
SMILES: CC
Mol. weight [g/mol]: 537.00

Physical Properties

Property code	Value	Unit	Source
gf	155.66	kJ/mol	Joback Method
hf	-939.23	kJ/mol	Joback Method
hfus	92.77	kJ/mol	Joback Method
hvap	100.37	kJ/mol	Joback Method
log10ws	-14.40		Crippen Method
logp	13.916		Crippen Method
mcvol	538.060	ml/mol	McGowan Method
pc	436.39	kPa	Joback Method
rinpol	3754.00		NIST Webbook
rinpol	3754.00		NIST Webbook
tb	1068.38	K	Joback Method
tc	1393.61	K	Joback Method
tf	528.98	K	Joback Method
vc	2.126	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1999.53	J/mol×K	1068.38	Joback Method
cpg	2036.87	J/mol×K	1122.58	Joback Method
cpg	2070.58	J/mol×K	1176.79	Joback Method
cpg	2101.02	J/mol×K	1230.99	Joback Method
cpg	2128.55	J/mol×K	1285.20	Joback Method
cpg	2153.52	J/mol×K	1339.40	Joback Method
cpg	2176.29	J/mol×K	1393.61	Joback Method
dvisc	0.0002482	Pa×s	528.98	Joback Method

dvisc	0.0000847	Pa×s	618.88	Joback Method
dvisc	0.0000379	Pa×s	708.78	Joback Method
dvisc	0.0000204	Pa×s	798.68	Joback Method
dvisc	0.0000124	Pa×s	888.58	Joback Method
dvisc	0.0000083	Pa×s	978.48	Joback Method
dvisc	0.0000059	Pa×s	1068.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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