

Heptyl octacosyl ether

Inchi: InChI=1S/C35H72O/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
InchiKey: GOKRFIPVTXGANL-UHFFFAOYSA-N
Formula: C35H72O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCCCCC
Mol. weight [g/mol]: 508.95

Physical Properties

Property code	Value	Unit	Source
gf	138.82	kJ/mol	Joback Method
hf	-897.95	kJ/mol	Joback Method
hfus	87.59	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Joback Method
log10ws	-13.56		Crippen Method
logp	13.136		Crippen Method
mvol	509.880	ml/mol	McGowan Method
pc	473.62	kPa	Joback Method
rinpol	3556.00		NIST Webbook
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tb	1022.62	K	Joback Method
tc	1307.47	K	Joback Method
tf	506.44	K	Joback Method
vc	2.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1860.76	J/molxK	1022.62	Joback Method
cpg	1894.69	J/molxK	1070.10	Joback Method
cpg	1925.72	J/molxK	1117.57	Joback Method
cpg	1954.07	J/molxK	1165.05	Joback Method
cpg	1979.96	J/molxK	1212.52	Joback Method
cpg	2003.63	J/molxK	1260.00	Joback Method
cpg	2025.29	J/molxK	1307.47	Joback Method
dvisc	0.0003357	Paxs	506.44	Joback Method

dvisc	0.0001153	Paxs	592.47	Joback Method
dvisc	0.0000519	Paxs	678.50	Joback Method
dvisc	0.0000280	Paxs	764.53	Joback Method
dvisc	0.0000171	Paxs	850.56	Joback Method
dvisc	0.0000114	Paxs	936.59	Joback Method
dvisc	0.0000082	Paxs	1022.62	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=U406400&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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