Docosyl heptyl ether

Inchi: InChI=1S/C29H60O/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27-29-3
InchiKey: LIMCJTPRXZHVLO-UHFFFAOYSA-N
Formula: C29H60O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOCCCCCCC
Mol. weight [g/mol]: 424.79

Physical Properties

Property code	Value	Unit	Source
gf	88.30	kJ/mol	Joback Method
hf	-774.11	kJ/mol	Joback Method
hfus	72.05	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	10.795		Crippen Method
mcvol	425.340	ml/mol	McGowan Method
pc	619.10	kPa	Joback Method
rinpol	2966.00		NIST Webbook
rinpol	2966.00		NIST Webbook
tb	885.34	K	Joback Method
tc	1090.98	K	Joback Method
tf	438.82	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1451.36	J/mol×K	885.34	Joback Method
cpg	1477.87	J/mol×K	919.61	Joback Method
cpg	1502.80	J/mol×K	953.89	Joback Method
cpg	1526.22	J/mol×K	988.16	Joback Method
cpg	1548.19	J/mol×K	1022.44	Joback Method
cpg	1568.78	J/mol×K	1056.71	Joback Method
cpg	1588.06	J/mol×K	1090.98	Joback Method
dvisc	0.0007935	Pa×s	438.82	Joback Method

dvisc	0.0002790	Pa×s	513.24	Joback Method
dvisc	0.0001278	Pa×s	587.66	Joback Method
dvisc	0.0000698	Pa×s	662.08	Joback Method
dvisc	0.0000431	Pa×s	736.50	Joback Method
dvisc	0.0000290	Pa×s	810.92	Joback Method
dvisc	0.0000209	Pa×s	885.34	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=U406397&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