Docosyl isobutyl ether

Inchi: InChI=1S/C26H54O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-27-2
InchiKey: PSWPJHLOGRHOIR-UHFFFAOYSA-N
Formula: C26H54O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 382.71

Physical Properties

Property code	Value	Unit	Source
gf	60.60	kJ/mol	Joback Method
hf	-717.47	kJ/mol	Joback Method
hfus	60.76	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	9.481		Crippen Method
mcvol	383.070	ml/mol	McGowan Method
pc	721.46	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
tb	816.26	K	Joback Method
tc	999.43	K	Joback Method
tf	390.01	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.01	J/mol×K	816.26	Joback Method
cpg	1361.16	J/mol×K	968.90	Joback Method
cpg	1341.85	J/mol×K	938.37	Joback Method
cpg	1321.42	J/mol×K	907.84	Joback Method
cpg	1299.83	J/mol×K	877.32	Joback Method
cpg	1277.04	J/mol×K	846.79	Joback Method
cpg	1379.40	J/mol×K	999.43	Joback Method
dvisc	0.0000300	Pa×s	816.26	Joback Method

dvisc	0.0000422	Pa×s	745.22	Joback Method
dvisc	0.0000638	Pa×s	674.18	Joback Method
dvisc	0.0001062	Pa×s	603.13	Joback Method
dvisc	0.0002027	Pa×s	532.09	Joback Method
dvisc	0.0004720	Pa×s	461.05	Joback Method
dvisc	0.0014951	Pa×s	390.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406331&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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