

octyl tetradecyl ether

Inchi: InChI=1S/C22H46O/c1-3-5-7-9-11-12-13-14-15-16-18-20-22-23-21-19-17-10-8-6-4-2/h3-22
InchiKey: OGJTVZHMxmmzch-UHFFFAOYSA-N
Formula: C22H46O
SMILES: CCCCCCCCCCCCCOCCCCCCCCC
Mol. weight [g/mol]: 326.60

Physical Properties

Property code	Value	Unit	Source
af	0.9911		Cheméo Relay (1.0)
gf	29.36	kJ/mol	Joback Method
hf	-628.32	kJ/mol	Cheméo Relay (1.0)
hfus	53.92	kJ/mol	Joback Method
hvap	108.83	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-8.05		Cheméo Relay (1.0)
logp	8.065		Crippen Method
mcvol	326.710	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
tb	597.41	K	Cheméo Relay (1.0)
tc	775.45	K	Cheméo Relay (1.0)
tf	288.65	K	Cheméo Relay (1.0)
vc	1.302	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.15	J/mol×K	725.18	Joback Method
cpg	1018.84	J/mol×K	752.93	Joback Method
cpg	1039.58	J/mol×K	780.68	Joback Method
cpg	1059.40	J/mol×K	808.43	Joback Method
cpg	1078.30	J/mol×K	836.19	Joback Method
cpg	1096.33	J/mol×K	863.94	Joback Method
cpg	1113.50	J/mol×K	891.69	Joback Method
dvisc	0.0019109	Pa×s	359.93	Joback Method

dvisc	0.0006985	Pa×s	420.80	Joback Method
dvisc	0.0003293	Pa×s	481.68	Joback Method
dvisc	0.0001837	Pa×s	542.55	Joback Method
dvisc	0.0001153	Pa×s	603.43	Joback Method
dvisc	0.0000789	Pa×s	664.30	Joback Method
dvisc	0.0000575	Pa×s	725.18	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=T999920728&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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