METHYL PENTADECYL ETHER

Inchi: InChI=1S/C16H34O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-2/h3-16H2,1-2H3
InchiKey: QTAFOTOCTOIEKW-UHFFFAOYSA-N
Formula: C16H34O
SMILES: CCCCCCCCCCCCCCCOC
Mol. weight [g/mol]: 242.45

Physical Properties

Property code	Value	Unit	Source
af	0.7634		Cheméo Relay (1.0)
gf	-21.16	kJ/mol	Joback Method
hf	-497.22	kJ/mol	Cheméo Relay (1.0)
hfus	38.38	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-6.49		Cheméo Relay (1.0)
logp	5.724		Crippen Method
mcvol	242.170	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
tb	555.47	K	Cheméo Relay (1.0)
tc	720.53	K	Cheméo Relay (1.0)
tf	293.37	K	Cheméo Relay (1.0)
vc	0.962	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.59	J/mol×K	587.90	Joback Method
cpg	662.46	J/mol×K	614.43	Joback Method
cpg	680.61	J/mol×K	640.97	Joback Method
cpg	698.07	J/mol×K	667.50	Joback Method
cpg	714.84	J/mol×K	694.03	Joback Method
cpg	730.94	J/mol×K	720.56	Joback Method
cpg	746.38	J/mol×K	747.10	Joback Method
dvisc	0.0033879	Pa×s	292.31	Joback Method

dvisc	0.0013014	Pa×s	341.57	Joback Method
dvisc	0.0006363	Pa×s	390.84	Joback Method
dvisc	0.0003651	Pa×s	440.11	Joback Method
dvisc	0.0002343	Pa×s	489.37	Joback Method
dvisc	0.0001631	Pa×s	538.63	Joback Method
dvisc	0.0001206	Pa×s	587.90	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7307520&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