ethyl 3-methylbutyl ether

Inchi: InChI=1S/C7H16O/c1-4-7(3)6-8-5-2/h7H,4-6H2,1-3H3
InchiKey: HMYXSLMGYNWZQR-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCOCC(C)CC
Mol. weight [g/mol]: 116.20
CAS: 628-04-6

Physical Properties

Property code	Value	Unit	Source
af	0.3828		Cheméo Relay (1.0)
gf	-99.38	kJ/mol	Joback Method
hf	-317.54	kJ/mol	Cheméo Relay (1.0)
hfus	11.55	kJ/mol	Joback Method
hvap	37.10	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-1.93		Cheméo Relay (1.0)
logp	2.069		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	378.76	K	Cheméo Relay (1.0)
tc	548.53	K	Cheméo Relay (1.0)
tf	149.42	K	Cheméo Relay (1.0)
vc	0.412	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.33	J/mol×K	381.54	Joback Method
cpg	230.17	J/mol×K	409.57	Joback Method
cpg	241.65	J/mol×K	437.59	Joback Method
cpg	252.77	J/mol×K	465.62	Joback Method
cpg	263.53	J/mol×K	493.64	Joback Method
cpg	273.94	J/mol×K	521.67	Joback Method
cpg	284.00	J/mol×K	549.69	Joback Method

dvisc	0.0068890	Pa×s	175.88	Joback Method
dvisc	0.0024170	Pa×s	210.16	Joback Method
dvisc	0.0011375	Pa×s	244.43	Joback Method
dvisc	0.0006444	Pa×s	278.71	Joback Method
dvisc	0.0004135	Pa×s	312.99	Joback Method
dvisc	0.0002896	Pa×s	347.26	Joback Method
dvisc	0.0002162	Pa×s	381.54	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628046&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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