2-(isobutyl-3-methylbutoxy)ethanol

Inchi: InChI=1S/C11H24O2/c1-9(2)5-6-13-11(8-12)7-10(3)4/h9-12H,5-8H2,1-4H3
InchiKey: GDFYQZHRZFIDNT-UHFFFAOYSA-N
Formula: C11H24O2
SMILES: CC(C)CCOC(CO)CC(C)C
Mol. weight [g/mol]: 188.31
CAS: 10086-50-7

Physical Properties

Property code	Value	Unit	Source
hfus	18.95	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Cheméo Relay (1.0)
logp	2.456		Crippen Method
mcvol	177.590	ml/mol	McGowan Method
tb	511.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.85	J/mol×K	564.36	Joback Method
cpg	471.48	J/mol×K	592.05	Joback Method
cpg	485.55	J/mol×K	619.75	Joback Method
cpg	499.04	J/mol×K	647.44	Joback Method
cpg	511.99	J/mol×K	675.14	Joback Method
cpg	524.39	J/mol×K	702.83	Joback Method
cpg	536.25	J/mol×K	730.53	Joback Method
dvisc	0.0901841	Pa×s	251.78	Joback Method
dvisc	0.0095251	Pa×s	303.88	Joback Method
dvisc	0.0019425	Pa×s	355.97	Joback Method
dvisc	0.0005945	Pa×s	408.07	Joback Method
dvisc	0.0002379	Pa×s	460.17	Joback Method
dvisc	0.0001147	Pa×s	512.26	Joback Method
dvisc	0.0000633	Pa×s	564.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.86993e+01
Coeff. B	-6.14570e+03
Coeff. C	-9.50310e+01
Temperature range (K), min.	428.82
Temperature range (K), max.	554.08

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.