

2-Propanol, 1,3-bis(3-methylbutoxy)-

Inchi:	InChI=1S/C13H28O3/c1-11(2)5-7-15-9-13(14)10-16-8-6-12(3)4/h11-14H,5-10H2,1-4H3
InchiKey:	ARRCKRNGGJHASO-UHFFFAOYSA-N
Formula:	C13H28O3
SMILES:	CC(C)CCOCC(O)COCCC(C)C
Mol. weight [g/mol]:	232.22

Physical Properties

Property code	Value	Unit	Source
hfus	25.32	kJ/mol	Joback Method
hvap	83.09	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	3.023		NCMS SOLV-DB
mcvol	211.640	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
tb	554.96	K	Cheméo Relay (1.0)
tc	717.51	K	Cheméo Relay (1.0)
tf	230.29	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	4.23160e+01
Coeff. B	1.16418e+00
Coeff. C	-5.01400e-04
Coeff. D	4.22000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.60917e+01
Coeff. B	3.61175e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	296.55
Temperature range (K), max.	558.86

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NCMS SOLV-DB:

<http://solvdb.ncms.org/common01.idc?solvno=00626788A>

Joback Method:

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

McGowan Method:

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

Crippen Method:

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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