

tripropylene glycol monobutyl ether

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H28O4/c1-5-6-7-15-9-12(3)17-10-13(4)16-8-11(2)14/h11-14H,5-10H2,1-4H

LORVPHHKJFSORQ-UHFFFAOYSA-N

C13H28O4

CCCCOCC(C)OCC(C)OCC(C)O

248.36

Physical Properties

Property code	Value	Unit	Source
af	0.8302		Cheméo Relay (1.0)
gf	-400.56	kJ/mol	Joback Method
hf	-904.95	kJ/mol	Cheméo Relay (1.0)
hfus	26.51	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-1.13		Cheméo Relay (1.0)
logp	1.994		Crippen Method
mcvol	217.510	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
tb	563.59	K	Cheméo Relay (1.0)
tc	706.85	K	Cheméo Relay (1.0)
tf	231.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.90	J/mol×K	654.96	Joback Method
cpg	633.48	J/mol×K	682.68	Joback Method
cpg	648.41	J/mol×K	710.40	Joback Method
cpg	662.71	J/mol×K	738.12	Joback Method
cpg	676.36	J/mol×K	765.84	Joback Method
cpg	689.36	J/mol×K	793.56	Joback Method
cpg	701.72	J/mol×K	821.28	Joback Method
dvisc	0.0091116	Pa×s	318.78	Joback Method
dvisc	0.0015819	Pa×s	374.81	Joback Method

dvisc	0.0004330	Pa×s	430.84	Joback Method
dvisc	0.0001597	Pa×s	486.87	Joback Method
dvisc	0.0000724	Pa×s	542.90	Joback Method
dvisc	0.0000380	Pa×s	598.93	Joback Method
dvisc	0.0000223	Pa×s	654.96	Joback Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Mutual Solubility and Lower Critical <https://www.doi.org/10.1021/je049635u>

Solution Temperature for Water + Organic Systems: 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>

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

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