1,1-Diisobutoxy-butane

Inchi:	InChI=1S/C12H26O2/c1-6-7-12(13-8-10(2)3)14-9-11(4)5/h10-12H,6-9H2,1-5H3
InchiKey:	UAPNJCMKUJQPBK-UHFFFAOYSA-N
Formula:	C12H26O2
SMILES:	CCCC(OCC(C)C)OCC(C)C
Mol. weight [g/mol]:	202.33
CAS:	13002-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-167.16	kJ/mol	Joback Method
hf	-571.29	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	45.96	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.458		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
tb	476.00 ± 5.00	K	NIST Webbook
tc	687.69	K	Joback Method
tf	224.46	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.91	J/mol×K	517.48	Joback Method
cpg	482.20	J/mol×K	545.85	Joback Method
cpg	498.88	J/mol×K	574.22	Joback Method
cpg	514.94	J/mol×K	602.58	Joback Method
cpg	530.40	J/mol×K	630.95	Joback Method
cpg	545.24	J/mol×K	659.32	Joback Method
cpg	559.48	J/mol×K	687.69	Joback Method
dvisc	0.0112913	Pa×s	224.46	Joback Method
dvisc	0.0026983	Pa×s	273.30	Joback Method

dvisc	0.0009952	Pa×s	322.13	Joback Method
dvisc	0.0004773	Pa×s	370.97	Joback Method
dvisc	0.0002716	Pa×s	419.81	Joback Method
dvisc	0.0001738	Pa×s	468.64	Joback Method
dvisc	0.0001210	Pa×s	517.48	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13002169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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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