

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/molxK	517.48	Joback Method
cpg	482.20	J/molxK	545.85	Joback Method
cpg	498.88	J/molxK	574.22	Joback Method
cpg	514.94	J/molxK	602.58	Joback Method
cpg	530.40	J/molxK	630.95	Joback Method
cpg	545.24	J/molxK	659.32	Joback Method
cpg	559.48	J/molxK	687.69	Joback Method
dvisc	0.0112913	Paxs	224.46	Joback Method
dvisc	0.0026983	Paxs	273.30	Joback Method

dvisc	0.0009952	Paxs	322.13	Joback Method
dvisc	0.0004773	Paxs	370.97	Joback Method
dvisc	0.0002716	Paxs	419.81	Joback Method
dvisc	0.0001738	Paxs	468.64	Joback Method
dvisc	0.0001210	Paxs	517.48	Joback Method

Sources

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

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
mccvol:	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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