

Diisobutyl (oxybis(ethane-2,1-diyl)) dicarbonate

Inchi:	InChI=1S/C14H26O7/c1-11(2)9-20-13(15)18-7-5-17-6-8-19-14(16)21-10-12(3)4/h11-12H
InchiKey:	LUALIVRVZDKYLW-UHFFFAOYSA-N
Formula:	C14H26O7
SMILES:	CC(C)COC(=O)OCCOCCOC(=O)OCC(C)C
Mol. weight [g/mol]:	306.35

Physical Properties

Property code	Value	Unit	Source
gf	-720.72	kJ/mol	Joback Method
hf	-1229.11	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	71.52	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.621		Crippen Method
mcvol	240.610	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook
tb	738.68	K	Joback Method
tc	920.55	K	Joback Method
tf	428.55	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.93	J/molxK	738.68	Joback Method
cpg	725.39	J/molxK	768.99	Joback Method
cpg	739.99	J/molxK	799.30	Joback Method
cpg	753.70	J/molxK	829.62	Joback Method
cpg	766.51	J/molxK	859.93	Joback Method
cpg	778.38	J/molxK	890.24	Joback Method
cpg	789.30	J/molxK	920.55	Joback Method
dvisc	0.0007081	Paxs	428.55	Joback Method

dvisc	0.0003499	Paxs	480.24	Joback Method
dvisc	0.0001983	Paxs	531.93	Joback Method
dvisc	0.0001242	Paxs	583.62	Joback Method
dvisc	0.0000840	Paxs	635.30	Joback Method
dvisc	0.0000602	Paxs	686.99	Joback Method
dvisc	0.0000453	Paxs	738.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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