

Isobutyl 2,5,8,11-tetraoxatridecan-13-yl carbonate

Inchi:	InChI=1S/C14H28O7/c1-13(2)12-21-14(15)20-11-10-19-9-8-18-7-6-17-5-4-16-3/h13H,4-
InchiKey:	IGXBUPBTGBNZKS-UHFFFAOYSA-N
Formula:	C14H28O7
SMILES:	COCCOCCOCCOCCOC(=O)OCC(C)C
Mol. weight [g/mol]:	308.37

Physical Properties

Property code	Value	Unit	Source
gf	-694.36	kJ/mol	Joback Method
hf	-1243.47	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	67.58	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	1.492		Crippen Method
mvol	244.910	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	707.67	K	Joback Method
tc	880.62	K	Joback Method
tf	415.85	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.76	J/molxK	707.67	Joback Method
cpg	732.04	J/molxK	736.50	Joback Method
cpg	747.57	J/molxK	765.32	Joback Method
cpg	762.30	J/molxK	794.15	Joback Method
cpg	776.21	J/molxK	822.97	Joback Method
cpg	789.28	J/molxK	851.80	Joback Method
cpg	801.48	J/molxK	880.62	Joback Method
dvisc	0.0005332	Paxs	415.85	Joback Method

dvisc	0.0002739	Paxs	464.49	Joback Method
dvisc	0.0001596	Paxs	513.12	Joback Method
dvisc	0.0001022	Paxs	561.76	Joback Method
dvisc	0.0000702	Paxs	610.40	Joback Method
dvisc	0.0000510	Paxs	659.03	Joback Method
dvisc	0.0000387	Paxs	707.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U378279&Units=SI

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
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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