

Carbonic acid, but-3-en-1-yl nonyl ester

Inchi:	InChI=1S/C14H26O3/c1-3-5-7-8-9-10-11-13-17-14(15)16-12-6-4-2/h4H,2-3,5-13H2,1H3
InchiKey:	NPPGNAIAAKJKTf-UHFFFAOYSA-N
Formula:	C14H26O3
SMILES:	C=CCCOC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	242.35

Physical Properties

Property code	Value	Unit	Source
gf	-184.08	kJ/mol	Joback Method
hf	-583.88	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.466		Crippen Method
mvol	217.130	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	615.11	K	Joback Method
tc	785.48	K	Joback Method
tf	340.17	K	Joback Method
vc	0.843	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.56	J/molxK	615.11	Joback Method
cpg	590.72	J/molxK	643.51	Joback Method
cpg	606.22	J/molxK	671.90	Joback Method
cpg	621.05	J/molxK	700.30	Joback Method
cpg	635.23	J/molxK	728.69	Joback Method
cpg	648.76	J/molxK	757.09	Joback Method
cpg	661.65	J/molxK	785.48	Joback Method
dvisc	0.0018627	Paxs	340.17	Joback Method

dvisc	0.0009096	Paxs	385.99	Joback Method
dvisc	0.0005171	Paxs	431.82	Joback Method
dvisc	0.0003277	Paxs	477.64	Joback Method
dvisc	0.0002249	Paxs	523.46	Joback Method
dvisc	0.0001640	Paxs	569.29	Joback Method
dvisc	0.0001253	Paxs	615.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383230&Units=SI
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

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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