

Carbonic acid, decyl hexadecyl ester

Inchi:	InChI=1S/C27H54O3/c1-3-5-7-9-11-13-14-15-16-17-18-20-22-24-26-30-27(28)29-25-23-
InchiKey:	MMJXTJZQLOLBPO-UHFFFAOYSA-N
Formula:	C27H54O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	426.72

Physical Properties

Property code	Value	Unit	Source
gf	-162.46	kJ/mol	Joback Method
hf	-977.63	kJ/mol	Joback Method
hfus	69.66	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	9.762		Crippen Method
mvol	404.600	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	915.87	K	Joback Method
tc	1128.23	K	Joback Method
tf	488.44	K	Joback Method
vc	1.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.92	J/molxK	915.87	Joback Method
cpg	1486.89	J/molxK	1092.83	Joback Method
cpg	1469.59	J/molxK	1057.44	Joback Method
cpg	1450.79	J/molxK	1022.05	Joback Method
cpg	1430.45	J/molxK	986.66	Joback Method
cpg	1408.51	J/molxK	951.26	Joback Method
cpg	1502.75	J/molxK	1128.23	Joback Method
dvisc	0.0000198	Paxs	915.87	Joback Method

dvisc	0.0000269	Paxs	844.63	Joback Method
dvisc	0.0000387	Paxs	773.39	Joback Method
dvisc	0.0000600	Paxs	702.15	Joback Method
dvisc	0.0001028	Paxs	630.92	Joback Method
dvisc	0.0002017	Paxs	559.68	Joback Method
dvisc	0.0004821	Paxs	488.44	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=U383165&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
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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