

Carbonic acid, decyl octadecyl ester

Inchi: InChI=1S/C29H58O3/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-22-24-26-28-32-29(30)31-
InchiKey: WQCRQTBXYVCRPB-UHFFFAOYSA-N
Formula: C29H58O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]: 454.77

Physical Properties

Property code	Value	Unit	Source
gf	-145.62	kJ/mol	Joback Method
hf	-1018.91	kJ/mol	Joback Method
hfus	74.84	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-10.89		Crippen Method
logp	10.542		Crippen Method
mcvol	432.780	ml/mol	McGowan Method
pc	633.52	kPa	Joback Method
rinpol	3115.00		NIST Webbook
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tb	961.63	K	Joback Method
tc	1194.59	K	Joback Method
tf	510.98	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1516.55	J/mol×K	961.63	Joback Method
cpg	1623.31	J/mol×K	1155.76	Joback Method
cpg	1605.67	J/mol×K	1116.93	Joback Method
cpg	1586.26	J/mol×K	1078.11	Joback Method
cpg	1564.98	J/mol×K	1039.28	Joback Method
cpg	1541.77	J/mol×K	1000.46	Joback Method
cpg	1639.23	J/mol×K	1194.59	Joback Method
dvisc	0.0000145	Pa×s	961.63	Joback Method

dvisc	0.0000197	Pa×s	886.52	Joback Method
dvisc	0.0000285	Pa×s	811.41	Joback Method
dvisc	0.0000445	Pa×s	736.30	Joback Method
dvisc	0.0000767	Pa×s	661.20	Joback Method
dvisc	0.0001521	Pa×s	586.09	Joback Method
dvisc	0.0003689	Pa×s	510.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U383167&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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