

Carbonic acid, decyl heptadecyl ester

Inchi: InChI=1S/C28H56O3/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27-31-28(29)30-26-
InchiKey: ALMUIXQXYATLFP-UHFFFAOYSA-N
Formula: C28H56O3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 440.74

Physical Properties

Property code	Value	Unit	Source
gf	-154.04	kJ/mol	Joback Method
hf	-998.27	kJ/mol	Joback Method
hfus	72.25	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	10.152		Crippen Method
mcvol	418.690	ml/mol	McGowan Method
pc	665.29	kPa	Joback Method
rinpol	3012.00		NIST Webbook
rinpol	3012.00		NIST Webbook
tb	938.75	K	Joback Method
tc	1160.75	K	Joback Method
tf	499.71	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1450.54	J/mol×K	938.75	Joback Method
cpg	1554.86	J/mol×K	1123.75	Joback Method
cpg	1537.38	J/mol×K	1086.75	Joback Method
cpg	1518.27	J/mol×K	1049.75	Joback Method
cpg	1497.47	J/mol×K	1012.75	Joback Method
cpg	1474.91	J/mol×K	975.75	Joback Method
cpg	1570.77	J/mol×K	1160.75	Joback Method
dvisc	0.0000169	Pa×s	938.75	Joback Method

dvisc	0.0000231	Pa×s	865.58	Joback Method
dvisc	0.0000333	Pa×s	792.40	Joback Method
dvisc	0.0000517	Pa×s	719.23	Joback Method
dvisc	0.0000889	Pa×s	646.06	Joback Method
dvisc	0.0001754	Pa×s	572.88	Joback Method
dvisc	0.0004222	Pa×s	499.71	Joback Method

Sources

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=U383166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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