

Carbonic acid, (1R)-(-)-menthyl octadecyl ester

Inchi: InChI=1S/C29H56O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-31-29(30)32-2
InchiKey: FYRACOOAGKJSSO-UHFFFAOYSA-N
Formula: C29H56O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]: 452.75

Physical Properties

Property code	Value	Unit	Source
gf	-139.03	kJ/mol	Joback Method
hf	-1010.55	kJ/mol	Joback Method
hfus	65.30	kJ/mol	Joback Method
hvap	91.14	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	9.862		Crippen Method
mvol	421.920	ml/mol	McGowan Method
pc	683.14	kPa	Joback Method
rinpol	3138.00		NIST Webbook
rinpol	3138.00		NIST Webbook
tb	971.40	K	Joback Method
tc	1192.89	K	Joback Method
tf	494.88	K	Joback Method
vc	1.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1522.32	J/molxK	971.40	Joback Method
cpg	1617.21	J/molxK	1155.97	Joback Method
cpg	1602.28	J/molxK	1119.06	Joback Method
cpg	1585.37	J/molxK	1082.14	Joback Method
cpg	1566.44	J/molxK	1045.23	Joback Method
cpg	1545.44	J/molxK	1008.31	Joback Method
cpg	1630.24	J/molxK	1192.89	Joback Method
dvisc	0.0000242	Paxs	971.40	Joback Method

dvisc	0.0000324	Paxs	891.98	Joback Method
dvisc	0.0000461	Paxs	812.56	Joback Method
dvisc	0.0000705	Paxs	733.14	Joback Method
dvisc	0.0001198	Paxs	653.72	Joback Method
dvisc	0.0002357	Paxs	574.30	Joback Method
dvisc	0.0005762	Paxs	494.88	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=U392446&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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