

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

Inchi:	InChI=1S/C27H52O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-27(28)30-26-22-2
InchiKey:	HVJGRMWSLAZGAW-UHFFFAOYSA-N
Formula:	C27H52O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]:	424.70

Physical Properties

Property code	Value	Unit	Source
gf	-155.87	kJ/mol	Joback Method
hf	-969.27	kJ/mol	Joback Method
hfus	60.11	kJ/mol	Joback Method
hvap	86.69	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.082		Crippen Method
mcvol	393.740	ml/mol	McGowan Method
pc	757.23	kPa	Joback Method
rinpol	2924.00		NIST Webbook
tb	925.64	K	Joback Method
tc	1133.44	K	Joback Method
tf	472.34	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.93	J/molxK	925.64	Joback Method
cpg	1413.54	J/molxK	960.27	Joback Method
cpg	1434.33	J/molxK	994.91	Joback Method
cpg	1453.33	J/molxK	1029.54	Joback Method
cpg	1470.56	J/molxK	1064.18	Joback Method
cpg	1486.08	J/molxK	1098.81	Joback Method
cpg	1499.91	J/molxK	1133.44	Joback Method
dvisc	0.0007352	Paxs	472.34	Joback Method
dvisc	0.0003053	Paxs	547.89	Joback Method

dvisc	0.0001569	Paxs	623.44	Joback Method
dvisc	0.0000931	Paxs	698.99	Joback Method
dvisc	0.0000612	Paxs	774.54	Joback Method
dvisc	0.0000433	Paxs	850.09	Joback Method
dvisc	0.0000324	Paxs	925.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392444&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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