

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

Inchi:	InChI=1S/C28H54O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-30-28(29)31-27-2
InchiKey:	GGPUVTCNPODVDU-UHFFFAOYSA-N
Formula:	C28H54O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]:	438.73

Physical Properties

Property code	Value	Unit	Source
gf	-147.45	kJ/mol	Joback Method
hf	-989.91	kJ/mol	Joback Method
hfus	62.70	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	9.472		Crippen Method
mvol	407.830	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	948.52	K	Joback Method
tc	1162.61	K	Joback Method
tf	483.61	K	Joback Method
vc	1.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1456.49	J/molxK	948.52	Joback Method
cpg	1479.34	J/molxK	984.20	Joback Method
cpg	1500.23	J/molxK	1019.88	Joback Method
cpg	1519.19	J/molxK	1055.57	Joback Method
cpg	1536.28	J/molxK	1091.25	Joback Method
cpg	1551.53	J/molxK	1126.93	Joback Method
cpg	1564.99	J/molxK	1162.61	Joback Method
dvisc	0.0006518	Paxs	483.61	Joback Method

dvisc	0.0002687	Paxs	561.10	Joback Method
dvisc	0.0001373	Paxs	638.58	Joback Method
dvisc	0.0000811	Paxs	716.07	Joback Method
dvisc	0.0000531	Paxs	793.55	Joback Method
dvisc	0.0000375	Paxs	871.04	Joback Method
dvisc	0.0000280	Paxs	948.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392445&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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