

Carbonic acid, decyl undecyl ester

Inchi:	InChI=1S/C22H44O3/c1-3-5-7-9-11-13-15-17-19-21-25-22(23)24-20-18-16-14-12-10-8-6
InchiKey:	AZZJAURDOGITTE-UHFFFAOYSA-N
Formula:	C22H44O3
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	356.58

Physical Properties

Property code	Value	Unit	Source
gf	-204.56	kJ/mol	Joback Method
hf	-874.43	kJ/mol	Joback Method
hfus	56.71	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	7.811		Crippen Method
mvol	334.150	ml/mol	McGowan Method
pc	917.72	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	801.47	K	Joback Method
tc	981.89	K	Joback Method
tf	432.09	K	Joback Method
vc	1.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.72	J/molxK	801.47	Joback Method
cpg	1156.41	J/molxK	951.82	Joback Method
cpg	1140.17	J/molxK	921.75	Joback Method
cpg	1122.90	J/molxK	891.68	Joback Method
cpg	1104.58	J/molxK	861.61	Joback Method
cpg	1085.20	J/molxK	831.54	Joback Method
cpg	1171.65	J/molxK	981.89	Joback Method
dvisc	0.0000418	Paxs	801.47	Joback Method

dvisc	0.0000563	Paxs	739.91	Joback Method
dvisc	0.0000801	Paxs	678.34	Joback Method
dvisc	0.0001223	Paxs	616.78	Joback Method
dvisc	0.0002049	Paxs	555.22	Joback Method
dvisc	0.0003906	Paxs	493.65	Joback Method
dvisc	0.0008948	Paxs	432.09	Joback Method

Sources

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=U383160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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