Carbonic acid, dodecyl 2-ethylhexyl ester

Inchi: InChI=1S/C21H42O3/c1-4-7-9-10-11-12-13-14-15-16-18-23-21(22)24-19-20(6-3)17-8-5-2
InchiKey: IACNBKMHIJAJGQ-UHFFFAOYSA-N
Formula: C21H42O3
SMILES: CCCCCCCCCCCCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 342.56

Physical Properties

Property code	Value	Unit	Source
gf	-215.42	kJ/mol	Joback Method
hf	-859.07	kJ/mol	Joback Method
hfus	50.60	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	7.277		Crippen Method
mcvol	320.060	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	778.15	K	Joback Method
tc	955.58	K	Joback Method
tf	405.82	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.15	J/mol×K	778.15	Joback Method
cpg	1093.32	J/mol×K	926.00	Joback Method
cpg	1077.28	J/mol×K	896.43	Joback Method
cpg	1060.26	J/mol×K	866.86	Joback Method
cpg	1042.25	J/mol×K	837.29	Joback Method
cpg	1023.21	J/mol×K	807.72	Joback Method
cpg	1108.40	J/mol×K	955.58	Joback Method
dvisc	0.0000444	Pa×s	778.15	Joback Method

dvisc	0.0000607	Pa×s	716.10	Joback Method
dvisc	0.0000882	Pa×s	654.04	Joback Method
dvisc	0.0001385	Pa×s	591.99	Joback Method
dvisc	0.0002417	Pa×s	529.93	Joback Method
dvisc	0.0004891	Pa×s	467.88	Joback Method
dvisc	0.0012278	Pa×s	405.82	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=U383139&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
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