Dodecyl decanoate

Inchi: InChI=1S/C22H44O2/c1-3-5-7-9-11-12-13-15-17-19-21-24-22(23)20-18-16-14-10-8-6-4-2
InchiKey: MNOODXPYABBZMC-UHFFFAOYSA-N
Formula: C22H44O2
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC
Mol. weight [g/mol]: 340.59

Physical Properties

Property code	Value	Unit	Source
af	1.0458		Cheméo Relay (1.0)
hf	-813.12	kJ/mol	Cheméo Relay (1.0)
hfus	55.52	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Cheméo Relay (1.0)
ie	9.72	eV	Cheméo Relay (1.0)
log10ws	-7.45		Cheméo Relay (1.0)
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2372.60		NIST Webbook
rinpol	2372.60		NIST Webbook
tb	606.77	K	Cheméo Relay (1.0)
tc	790.09	K	Cheméo Relay (1.0)
tf	298.21	K	Cheméo Relay (1.0)
vc	1.294	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.01	J/mol×K	779.05	Joback Method
cpg	1051.60	J/mol×K	808.49	Joback Method
cpg	1071.17	J/mol×K	837.93	Joback Method
cpg	1089.74	J/mol×K	867.37	Joback Method
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1139.78	J/mol×K	955.69	Joback Method

dvisc	0.0013386	Pa×s	409.86	Joback Method
dvisc	0.0005575	Pa×s	471.39	Joback Method
dvisc	0.0002843	Pa×s	532.92	Joback Method
dvisc	0.0001666	Pa×s	594.45	Joback Method
dvisc	0.0001080	Pa×s	655.99	Joback Method
dvisc	0.0000754	Pa×s	717.52	Joback Method
dvisc	0.0000557	Pa×s	779.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42231505&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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