Decyl laurate

Other names: Decyl dodecanoate
Inchi: InChI=1S/C22H44O2/c1-3-5-7-9-11-13-14-16-18-20-22(23)24-21-19-17-15-12-10-8-6-4-2
InchiKey: RAPXDXJBAYUBHI-UHFFFAOYSA-N
Formula: C22H44O2
SMILES: CCCCCCCCCCCC(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 340.58
CAS: 36528-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2356.00		NIST Webbook
rinpol	2371.70		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
vc	1.292	m3/kmol	Joback Method

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
hfust	63.67	kJ/mol	293.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36528286&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust: Enthalpy of fusion at a given temperature
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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