octyl docosanoate

Inchi:	InChI=1S/C30H60O2/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-28-30(
InchiKey:	MWSXIWIELAIOBE-UHFFFAOYSA-N
Formula:	C30H60O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	452.80
CAS:	5979-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-32.20	kJ/mol	Joback Method
hf	-907.33	kJ/mol	Joback Method
hfus	76.24	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-11.24		Crippen Method
logp	10.712		Crippen Method
mcvol	441.000	ml/mol	McGowan Method
pc	609.06	kPa	Joback Method
rinpol	3160.05		NIST Webbook
tb	962.09	K	Joback Method
tc	1195.84	K	Joback Method
tf	500.02	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.95	J/mol×K	962.09	Joback Method
cpg	1575.26	J/mol×K	1001.05	Joback Method
cpg	1599.65	J/mol×K	1040.01	Joback Method
cpg	1622.22	J/mol×K	1078.97	Joback Method
cpg	1643.07	J/mol×K	1117.92	Joback Method
cpg	1662.31	J/mol×K	1156.88	Joback Method
cpg	1680.03	J/mol×K	1195.84	Joback Method
dvisc	0.0004872	Pa×s	500.02	Joback Method

dvisc	0.0001913	Pa×s	577.03	Joback Method
dvisc	0.0000936	Pa×s	654.04	Joback Method
dvisc	0.0000532	Pa×s	731.05	Joback Method
dvisc	0.0000337	Pa×s	808.07	Joback Method
dvisc	0.0000231	Pa×s	885.08	Joback Method
dvisc	0.0000168	Pa×s	962.09	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=C5979986&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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