

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:	CCCCCCCCCCCCCCCCCCCC(=O)CCCCCCCC
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001913	Paxs	577.03	Joback Method
dvisc	0.0000936	Paxs	654.04	Joback Method
dvisc	0.0000532	Paxs	731.05	Joback Method
dvisc	0.0000337	Paxs	808.07	Joback Method
dvisc	0.0000231	Paxs	885.08	Joback Method
dvisc	0.0000168	Paxs	962.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5979986&Units=SI

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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