

Stearyl isooctanoate

Inchi:	InChI=1S/C26H52O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-26(27)28-24-21-18
InchiKey:	SJIDAAGFCNIAJP-UHFFFAOYSA-N
Formula:	C26H52O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCCCC(C)C
Mol. weight [g/mol]:	396.69

Physical Properties

Property code	Value	Unit	Source
gf	-68.32	kJ/mol	Joback Method
hf	-830.05	kJ/mol	Joback Method
hfus	62.36	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.008		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinpol	2660.00		NIST Webbook
tb	870.13	K	Joback Method
tc	1066.30	K	Joback Method
tf	439.94	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.77	J/molxK	870.13	Joback Method
cpg	1308.62	J/molxK	902.82	Joback Method
cpg	1330.12	J/molxK	935.52	Joback Method
cpg	1350.31	J/molxK	968.21	Joback Method
cpg	1369.26	J/molxK	1000.91	Joback Method
cpg	1387.01	J/molxK	1033.60	Joback Method
cpg	1403.60	J/molxK	1066.30	Joback Method
dvisc	0.0009974	Paxs	439.94	Joback Method
dvisc	0.0003640	Paxs	511.64	Joback Method

dvisc	0.0001702	Paxs	583.34	Joback Method
dvisc	0.0000940	Paxs	655.04	Joback Method
dvisc	0.0000583	Paxs	726.73	Joback Method
dvisc	0.0000395	Paxs	798.43	Joback Method
dvisc	0.0000285	Paxs	870.13	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=R44544&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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