

hexyl eicosanoate

Inchi:	InChI=1S/C26H52O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-26(27)28-
InchiKey:	MPLBHUPXLJXOLF-UHFFFAOYSA-N
Formula:	C26H52O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	396.69

Physical Properties

Property code	Value	Unit	Source
gf	-65.88	kJ/mol	Joback Method
hf	-824.77	kJ/mol	Joback Method
hfus	65.88	kJ/mol	Joback Method
hvap	82.63	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	9.152		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpol	2765.80		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2765.80		NIST Webbook
tb	870.57	K	Joback Method
tc	1067.44	K	Joback Method
tf	454.94	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.37	J/molxK	870.57	Joback Method
cpg	1387.08	J/molxK	1034.63	Joback Method
cpg	1369.24	J/molxK	1001.82	Joback Method
cpg	1350.19	J/molxK	969.01	Joback Method
cpg	1329.90	J/molxK	936.19	Joback Method
cpg	1308.31	J/molxK	903.38	Joback Method
cpg	1403.78	J/molxK	1067.44	Joback Method

dvisc	0.0000311	Paxs	870.57	Joback Method
dvisc	0.0000424	Paxs	801.30	Joback Method
dvisc	0.0000614	Paxs	732.03	Joback Method
dvisc	0.0000959	Paxs	662.75	Joback Method
dvisc	0.0001664	Paxs	593.48	Joback Method
dvisc	0.0003338	Paxs	524.21	Joback Method
dvisc	0.0008279	Paxs	454.94	Joback Method

Sources

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=R437839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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