Eicosyl hexanoate

Inchi: InChI=1S/C26H52O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-25-28-26(2
InchiKey: KWCMZXYKOALZSP-UHFFFAOYSA-N
Formula: C26H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC
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	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook
rinpol	2771.00		NIST Webbook
rinpol	2771.00		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/mol×K	870.57	Joback Method
cpg	1387.08	J/mol×K	1034.63	Joback Method
cpg	1369.24	J/mol×K	1001.82	Joback Method
cpg	1350.19	J/mol×K	969.01	Joback Method
cpg	1329.90	J/mol×K	936.19	Joback Method
cpg	1308.31	J/mol×K	903.38	Joback Method

cpg	1403.78	J/mol×K	1067.44	Joback Method
dvisc	0.0000311	Pa×s	870.57	Joback Method
dvisc	0.0000424	Pa×s	801.30	Joback Method
dvisc	0.0000614	Pa×s	732.03	Joback Method
dvisc	0.0000959	Pa×s	662.75	Joback Method
dvisc	0.0001664	Pa×s	593.48	Joback Method
dvisc	0.0003338	Pa×s	524.21	Joback Method
dvisc	0.0008279	Pa×s	454.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R399287&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.