pentacosyl hexanoate

Inchi: InChI=1S/C31H62O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: KPIFJVLEGYFLOK-UHFFFAOYSA-N
Formula: C31H62O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]: 466.82

Physical Properties

Property code	Value	Unit	Source
gf	-23.78	kJ/mol	Joback Method
hf	-927.97	kJ/mol	Joback Method
hfus	78.83	kJ/mol	Joback Method
hvap	93.76	kJ/mol	Joback Method
log10ws	-11.66		Crippen Method
logp	11.102		Crippen Method
mcvol	455.090	ml/mol	McGowan Method
pc	581.20	kPa	Joback Method
rinpol	3268.87		NIST Webbook
rinpol	3268.87		NIST Webbook
tb	984.97	K	Joback Method
tc	1231.24	K	Joback Method
tf	511.29	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1615.90	J/mol×K	984.97	Joback Method
cpg	1732.71	J/mol×K	1190.19	Joback Method
cpg	1713.09	J/mol×K	1149.15	Joback Method
cpg	1691.73	J/mol×K	1108.10	Joback Method
cpg	1668.49	J/mol×K	1067.06	Joback Method
cpg	1643.25	J/mol×K	1026.01	Joback Method
cpg	1750.69	J/mol×K	1231.24	Joback Method
dvisc	0.0000144	Pa×s	984.97	Joback Method

dvisc	0.0000198	Pa×s	906.02	Joback Method
dvisc	0.0000289	Pa×s	827.08	Joback Method
dvisc	0.0000457	Pa×s	748.13	Joback Method
dvisc	0.0000806	Pa×s	669.18	Joback Method
dvisc	0.0001655	Pa×s	590.24	Joback Method
dvisc	0.0004241	Pa×s	511.29	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=R437993&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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