heptacosyl hexanoate

Inchi: InChI=1S/C33H66O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: QBALSVJGWNGXBA-UHFFFAOYSA-N
Formula: C33H66O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]: 494.88

Physical Properties

Property code	Value	Unit	Source
gf	-6.94	kJ/mol	Joback Method
hf	-969.25	kJ/mol	Joback Method
hfus	84.01	kJ/mol	Joback Method
hvap	98.21	kJ/mol	Joback Method
log10ws	-12.50		Crippen Method
logp	11.882		Crippen Method
mcvol	483.270	ml/mol	McGowan Method
pc	530.91	kPa	Joback Method
rinpol	3469.77		NIST Webbook
tb	1030.73	K	Joback Method
tc	1306.79	K	Joback Method
tf	533.83	K	Joback Method
vc	1.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1750.75	J/mol×K	1030.73	Joback Method
cpg	1875.18	J/mol×K	1260.78	Joback Method
cpg	1854.77	J/mol×K	1214.77	Joback Method
cpg	1832.30	J/mol×K	1168.76	Joback Method
cpg	1807.60	J/mol×K	1122.75	Joback Method
cpg	1780.48	J/mol×K	1076.74	Joback Method
cpg	1893.74	J/mol×K	1306.79	Joback Method
dvisc	0.0000105	Pa×s	1030.73	Joback Method
dvisc	0.0000144	Pa×s	947.91	Joback Method

dvisc	0.0000211	Pa×s	865.10	Joback Method
dvisc	0.0000336	Pa×s	782.28	Joback Method
dvisc	0.0000595	Pa×s	699.46	Joback Method
dvisc	0.0001232	Pa×s	616.65	Joback Method
dvisc	0.0003193	Pa×s	533.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437804&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