2-Hexyl heptadecanoate

Inchi: InChI=1S/C23H46O2/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-21-23(24)25-22(3)20-7
InchiKey: OHBZPLUUJYQIPI-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCC(=O)OC(C)CCCC
Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-93.58	kJ/mol	Joback Method
hf	-768.13	kJ/mol	Joback Method
hfus	54.59	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.980		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook
tb	801.49	K	Joback Method
tc	982.25	K	Joback Method
tf	406.13	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.96	J/mol×K	801.49	Joback Method
cpg	1115.11	J/mol×K	831.62	Joback Method
cpg	1135.16	J/mol×K	861.74	Joback Method
cpg	1154.15	J/mol×K	891.87	Joback Method
cpg	1172.09	J/mol×K	921.99	Joback Method
cpg	1189.04	J/mol×K	952.12	Joback Method
cpg	1205.01	J/mol×K	982.25	Joback Method
dvisc	0.0014705	Pa×s	406.13	Joback Method

dvisc	0.0005460	Pa×s	472.02	Joback Method
dvisc	0.0002584	Pa×s	537.92	Joback Method
dvisc	0.0001440	Pa×s	603.81	Joback Method
dvisc	0.0000900	Pa×s	669.70	Joback Method
dvisc	0.0000612	Pa×s	735.60	Joback Method
dvisc	0.0000444	Pa×s	801.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422798&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

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