

3-Hexyl 3,14-dimethylpentadecanoate

Inchi:	InChI=1S/C23H46O2/c1-6-16-22(7-2)25-23(24)19-21(5)18-15-13-11-9-8-10-12-14-17-20
InchiKey:	IHAVEWNYCCTFTN-UHFFFAOYSA-N
Formula:	C23H46O2
SMILES:	CCCC(CC)OC(=O)CC(C)CCCCCCCCCCC(C)C
Mol. weight [g/mol]:	354.61

Physical Properties

Property code	Value	Unit	Source
gf	-98.46	kJ/mol	Joback Method
hf	-778.69	kJ/mol	Joback Method
hfus	47.54	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.691		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	800.61	K	Joback Method
tc	982.44	K	Joback Method
tf	376.13	K	Joback Method
vc	1.329	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.83	J/molxK	800.61	Joback Method
cpg	1190.29	J/molxK	952.13	Joback Method
cpg	1173.33	J/molxK	921.83	Joback Method
cpg	1155.33	J/molxK	891.52	Joback Method
cpg	1136.27	J/molxK	861.22	Joback Method
cpg	1116.12	J/molxK	830.91	Joback Method
cpg	1206.25	J/molxK	982.44	Joback Method
dvisc	0.0000375	Paxs	800.61	Joback Method

dvisc	0.0000536	Paxs	729.86	Joback Method
dvisc	0.0000828	Paxs	659.12	Joback Method
dvisc	0.0001420	Paxs	588.37	Joback Method
dvisc	0.0002823	Paxs	517.62	Joback Method
dvisc	0.0006975	Paxs	446.88	Joback Method
dvisc	0.0024223	Paxs	376.13	Joback Method

Sources

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=R422812&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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