hexyl 7-octenoate

Inchi: InChI=1S/C14H26O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h3H,1,4-13H2,2H3
InchiKey: CFVNOTDKULCDEH-UHFFFAOYSA-N
Formula: C14H26O2
SMILES: C=CCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-79.08	kJ/mol	Joback Method
hf	-451.66	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	55.24	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
ripol	1838.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	592.69	K	Joback Method
tc	763.14	K	Joback Method
tf	317.94	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.69	J/mol×K	592.69	Joback Method
cpg	620.91	J/mol×K	734.73	Joback Method
cpg	607.19	J/mol×K	706.32	Joback Method
cpg	592.82	J/mol×K	677.92	Joback Method
cpg	577.79	J/mol×K	649.51	Joback Method

cpg	562.09	J/mol×K	621.10	Joback Method
cpg	634.00	J/mol×K	763.14	Joback Method
dvisc	0.0001590	Pa×s	592.69	Joback Method
dvisc	0.0002089	Pa×s	546.90	Joback Method
dvisc	0.0002885	Pa×s	501.11	Joback Method
dvisc	0.0004251	Pa×s	455.31	Joback Method
dvisc	0.0006832	Pa×s	409.52	Joback Method
dvisc	0.0012373	Pa×s	363.73	Joback Method
dvisc	0.0026588	Pa×s	317.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313674&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume