

5-hexenyl octanoate

Inchi:	InChI=1S/C14H26O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h4H,2-3,5-13H2,1H3
InchiKey:	PQKICODUSVBEAN-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	C=CCCCCOC(=O)CCCCCCC
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	1851.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1845.00		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/molxK	592.69	Joback Method
cpg	562.09	J/molxK	621.10	Joback Method
cpg	577.79	J/molxK	649.51	Joback Method
cpg	592.82	J/molxK	677.92	Joback Method
cpg	607.19	J/molxK	706.32	Joback Method

cpg	620.91	J/mol×K	734.73	Joback Method
cpg	634.00	J/mol×K	763.14	Joback Method
dvisc	0.0026588	Paxs	317.94	Joback Method
dvisc	0.0012373	Paxs	363.73	Joback Method
dvisc	0.0006832	Paxs	409.52	Joback Method
dvisc	0.0004251	Paxs	455.31	Joback Method
dvisc	0.0002885	Paxs	501.11	Joback Method
dvisc	0.0002089	Paxs	546.90	Joback Method
dvisc	0.0001590	Paxs	592.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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